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PDB ID	:	8H33
EMDB ID	:	EMD-34449
Title	:	Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 tetrameric complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-07
Resolution	:	7.86 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 7.86 Å.

Sidechain outliers

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



154315

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

3826

Mol	Chain	Length	Quality of chain					
1	А	623	61%	27%	• 10%			
1	В	623	60%	27%	• 11%			
1	G	623	60%	27%	• 10%			
1	J	623	61%	26%	• 11%			
2	D	121	47% 25%	6 ••	26%			
2	Е	121	40% 28%	5% •	26%			
2	K	121	41% 27%	••	26%			
2	L	121	38% 32%	••	26%			



Mol	Chain	Length	Quality of c	hain	
3	С	776	60%	29%	• 7%
3	F	776	59%	29%	• 7%
3	Н	776	58%	31%	• 7%
3	Ι	776	59%	30%	• 7%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 43620 atoms, of which 72 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		Atoms					AltConf	Trace
1	Δ	562	Total	С	Η	Ν	Ο	S	0	0
1	Л	502	4473	2842	18	746	832	35	0	0
1	В	557	Total	С	Η	Ν	Ο	S	0	0
	D		4464	2839	18	737	834	36	0	0
1	C	562	Total	С	Η	Ν	Ο	S	0	0
1	I G	502	4438	2820	18	743	823	34	0	0
1	1 T	555	Total	С	Η	Ν	Ο	S	0	0
J	J	555	4482	2855	18	740	832	37	0	0

• Molecule 1 is a protein called Kelch repeat and BTB domain-containing protein 2.

• Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues		At	oms			AltConf	Trace
2	а	80	Total	С	Ν	0	S	0	0
2		03	695	443	121	124	7	0	0
2	K	80	Total	С	Ν	Ο	\mathbf{S}	0	0
		09	737	466	135	127	9		0
0	т	80	Total	С	Ν	0	S	0	0
		89	737	466	135	127	9	0	0
0	F	80	Total	С	Ν	0	S	0	0
	Ľ	89	737	466	135	127	9	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P62877
D	-11	HIS	-	expression tag	UNP P62877
D	-10	HIS	-	expression tag	UNP P62877
D	-9	HIS	-	expression tag	UNP P62877
D	-8	HIS	-	expression tag	UNP P62877
D	-7	HIS	-	expression tag	UNP P62877
D	-6	GLU	-	expression tag	UNP P62877
D	-5	ASN	-	expression tag	UNP P62877
D	-4	LEU	-	expression tag	UNP P62877



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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	TYR	-	expression tag	UNP P62877
D	-2	PHE	-	expression tag	UNP P62877
D	-1	GLN	-	expression tag	UNP P62877
D	0	GLY	-	expression tag	UNP P62877
K	-12	HIS	-	expression tag	UNP P62877
K	-11	HIS	-	expression tag	UNP P62877
K	-10	HIS	-	expression tag	UNP P62877
K	-9	HIS	-	expression tag	UNP P62877
K	-8	HIS	-	expression tag	UNP P62877
K	-7	HIS	-	expression tag	UNP P62877
K	-6	GLU	-	expression tag	UNP P62877
K	-5	ASN	-	expression tag	UNP P62877
K	-4	LEU	-	expression tag	UNP P62877
K	-3	TYR	-	expression tag	UNP P62877
K	-2	PHE	-	expression tag	UNP P62877
K	-1	GLN	-	expression tag	UNP P62877
K	0	GLY	-	expression tag	UNP P62877
L	-12	HIS	-	expression tag	UNP P62877
L	-11	HIS	-	expression tag	UNP P62877
L	-10	HIS	-	expression tag	UNP P62877
L	-9	HIS	-	expression tag	UNP P62877
L	-8	HIS	-	expression tag	UNP P62877
L	-7	HIS	-	expression tag	UNP P62877
L	-6	GLU	-	expression tag	UNP P62877
L	-5	ASN	-	expression tag	UNP P62877
L	-4	LEU	-	expression tag	UNP P62877
L	-3	TYR	-	expression tag	UNP P62877
L	-2	PHE	-	expression tag	UNP P62877
L	-1	GLN	-	expression tag	UNP P62877
L	0	GLY	-	expression tag	UNP P62877
Е	-12	HIS	-	expression tag	UNP P62877
Е	-11	HIS	-	expression tag	UNP P62877
Е	-10	HIS	-	expression tag	UNP P62877
Е	-9	HIS	-	expression tag	UNP P62877
Е	-8	HIS	-	expression tag	UNP P62877
Е	-7	HIS	-	expression tag	UNP P62877
Е	-6	GLU	-	expression tag	UNP P62877
Е	-5	ASN	-	expression tag	UNP P62877
Е	-4	LEU	-	expression tag	UNP P62877
Е	-3	TYR	-	expression tag	UNP P62877
Е	-2	PHE	-	expression tag	UNP P62877
Е	-1	GLN	-	expression tag	UNP P62877

d fa α ntin



Chain	Residue	Modelled	Actual	Comment	Reference
Ε	0	GLY	-	expression tag	UNP P62877

• Molecule 3 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	720	Total	С	Ν	Ο	S	0	0
5	Ľ	120	5651	3540	1003	1071	37	0	0
3	Ц	720	Total	С	Ν	Ο	\mathbf{S}	0	0
5	11	720	5719	3589	1019	1073	38	0	0
2	т	720	Total	С	Ν	Ο	S	0	0
5	1	720	5722	3585	1013	1086	38	0	0
3	С	720	Total	С	Ν	Ο	S	0	0
J	U	120	5753	3613	1022	1081	37		0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	TRP	-	expression tag	UNP Q13618
F	-6	SER	-	expression tag	UNP Q13618
F	-5	HIS	-	expression tag	UNP Q13618
F	-4	PRO	-	expression tag	UNP Q13618
F	-3	GLN	-	expression tag	UNP Q13618
F	-2	PHE	-	expression tag	UNP Q13618
F	-1	GLU	-	expression tag	UNP Q13618
F	0	LYS	-	expression tag	UNP Q13618
Н	-7	TRP	-	expression tag	UNP Q13618
H	-6	SER	-	expression tag	UNP Q13618
Н	-5	HIS	-	expression tag	UNP Q13618
Н	-4	PRO	-	expression tag	UNP Q13618
Н	-3	GLN	-	expression tag	UNP Q13618
Н	-2	PHE	-	expression tag	UNP Q13618
Н	-1	GLU	-	expression tag	UNP Q13618
Н	0	LYS	-	expression tag	UNP Q13618
Ι	-7	TRP	-	expression tag	UNP Q13618
Ι	-6	SER	-	expression tag	UNP Q13618
Ι	-5	HIS	-	expression tag	UNP Q13618
Ι	-4	PRO	-	expression tag	UNP Q13618
Ι	-3	GLN	-	expression tag	UNP Q13618
Ι	-2	PHE	-	expression tag	UNP Q13618
Ι	-1	GLU	-	expression tag	UNP Q13618
Ι	0	LYS	-	expression tag	UNP Q13618
С	-7	TRP	-	expression tag	UNP Q13618



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Chain	Residue	Modelled	Actual	Comment	Reference				
С	-6	SER	-	expression tag	UNP Q13618				
С	-5	HIS	-	expression tag	UNP Q13618				
С	-4	PRO	-	expression tag	UNP Q13618				
С	-3	GLN	-	expression tag	UNP Q13618				
С	-2	PHE	-	expression tag	UNP Q13618				
С	-1	GLU	-	expression tag	UNP Q13618				
C	0	LYS	-	expression tag	UNP Q13618				

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	D	3	Total Zn 3 3	0
4	K	3	Total Zn 3 3	0
4	L	3	Total Zn 3 3	0
4	Ε	3	Total Zn 3 3	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Kelch repeat and BTB domain-containing protein 2



• Molecule 1: Kelch repeat and BTB domain-containing protein 2







• Molecule 1: Kelch repeat and BTB domain-containing protein 2



 \bullet Molecule 1: Kelch repeat and BTB domain-containing protein 2



V2 42 42 12 12 12 12 12 12 12 12 12 12 12 12 12	8252 M2554 M2554 M265 M265 M263 M268 M268 M268 M268 M268 M268 M268 M268	8275 8275 7288 7288 7288 8289 8289 8289 8289 8289	P301 P302 P302 P302 D304 L305 I318	A321 G322 G323 G323 U325 P326	LYS LYS THR ASN HIS
SER LYS SER LYS LYS LEU CLN THR ALA ALA	R345 R349 F350 F353 F353 F353 F353 F353 F365 F365 F365	8374 1375 1375 1375 0378 0378 1379 1383 1385 1385 1385 1385	VAL GLY GLV GLU LEU ASN ARG ARG	T398 T398 V399 8400 R401 7402 V409 4409	5413 P414 L415 P416 C417
A418 W419 V425 V425 I431 I431 M434 T435	1436 1436 1438 1438 1448 1449 1449 1455 1455 1455 1455 1455 1455	6476 L477 HIS HILE HILE ALA ALA SER SER GLY CLE LEC	PRO SER GLY THR VAL ASP GLY SER	S496 E500 D522 V525	
M538 R539 Y548 Y549 Q553 D555	L558 4661 8664 4664 4656 1656 1656 1656 8573 8573 8577 8577 8577 8577 8577 8577	E592 E593 E594 F80 PR0 PR0 LEU LEU FHE LEU THR	ASP GLY GLU GLU PHE GLU LEU	ASP GLV GLU MET VAL ALA LEU PRO	VAL
• Molecule 2:	E3 ubiquitin-protein l	igase RBX1			
Chain D:	47%	25%		26%	
HTS HTS HTS HTS HTS HTS GLU CLEU TYR	PHE GLY GLY MET MET ALA ALA ALA ALA ALA ALA ASP VAL ASP PRO SER FRO SER FRO SER FRO	855 617 617 617 617 617 721 721 722 725 725 725 725 725 725	W27 N28 A29 V30 A31 L32 W33 A34	N35 V38 I44 I49	
C68 W72 W72 C75 N76 H77 184	866 866 467 168 188 188 188 188 188 198 197 196 196 196 196 196 196 196 196 196 196				
• Molecule 2:	E3 ubiquitin-protein l	igase RBX1			
Chain K:	41%	27%		26%	
HIS HIS HIS HIS HIS AIN AIN LEU LEU TYR	PHE GLN GLN MET MET ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY	858 811 811 811 811 812 823 825 823 825 825 825 825	W27 N28 A29 A31 A31 M35	V38 N41 C42 R46 N47 H48	L52 C53 154 E55
CB6 457 457 458 469 461 461 461 461 410 410 410 410 410 410 410 410 410 41	C66 W72 W72 C75 C75 C75 C75 C75 C75 C75 C75 C41A ALLA ALLA ALLA ALLA ALLA ALLA ALLA A	C94 600 100 100 100 100 100 100 100 100 100	W27 N28 A29 A31 A31	V38 N41 C42 R46 N47 H48	L52 C53 154 E55
Image: Second state sta	開きる員名名名 日本	tigase RBX1	W27 N28 A29 A31 A31	V38 N41 C42 R46 N47 H48	L52 C53 154 E55
HERERERE SERVERE Molecule 2: Chain L:	 第一部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部部	Image: Second state Image: Second st	• • N28 A29 A31 A31 B85	26%	1.62 063 1.64 1.64
H H H H H H H H H H H H H H H H H H H	8 5 5 1	Market	W27 W27 N28 N29 A31 A31 A31 A31 A34 M34	W35 103 W41 104 W41 104 W41 104 W44 10	N47 N47 H48 152 CG3 CG3 CG3 CG3 CG3 CG3 CG3 CG3 CG3 CG3
Image: Second state sta	80 1	1 1 <td>N27 N28 A29 V30 V30 A31 A31 A31 A34 A34</td> <td>138 144 144 144 144 144 144 144 144 144 14</td> <td>M40 M47 H48 H48 L52 L52 L52</td>	N27 N28 A29 V30 V30 A31 A31 A31 A34 A34	138 144 144 144 144 144 144 144 144 144 14	M40 M47 H48 H48 L52 L52 L52
Image:	# 3 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Image: Second system Image: Second system <td< td=""><td>W27 N28 N29 N30 N31 N31 N33 N33 N34 N34</td><td>138 138 138 141 141 141 141 141 141 141 141 141</td><td>N47 N47 H48 L52 L52 L52 L52 L52 L52</td></td<>	W27 N28 N29 N30 N31 N31 N33 N33 N34 N34	138 138 138 141 141 141 141 141 141 141 141 141	N47 N47 H48 L52 L52 L52 L52 L52 L52
H H H H H H H H H H H H H H H H H H H	Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of the second state Image: Solution of th	$\frac{1}{2} = \frac{1}{2} + \frac{1}$	V27 V28 V33 V33 V33 V33 V33 V33 V33 V33 V33 V3	26%	M40 M47 L92 H48 1.62 0.53 L52 1.64 1.64 L52 1.64 1.64

WORLDWIDE PROTEIN DATA BANK



• Molecule 3: Cullin-3

Cha	in	F	?:											59	%															29	%					•		7'	%	1			
TRP SER HIS	PRO	GLN PHE	GLU	LYS	SER	ASN	LEU SER	LYS	GLY	THR	SER	ARG	LYS	ASP	LYS	MET	ARG	ARG	ALA	PHE	PRO MET	THR	M25	E 10		N48		104	Y74	<u> 77</u>	1	186		OGN	L102		e TT h	M116	V117	M118	1118 R120	-	L123 M124
D127 R128		V139 V140	N141	L142	L144	2	R148 D149	Q150		R153	L166	D167	M168	1169	A182	I183			L193		R198	V200	Y201	E202 E203	D204	F205	E206	A20/ P208		M212	5213 A214		F217	M219	E220		K223	r 224 L225	-	A230	E238		N242
1245 E246 R247	V248	SORE SORE	T256	E257 E260	P259		V263 V264	E265	R266	E267	1269 1269	S270	K271	H272	1276	-	S282	VORE	H286	M287		M299	Y300	K301	V306		K311	L328		K336 N227	P338	V339	D340	1342 1342	-	L345	L340	K349	S350	R351	F355	L356	L357 E358
D363 R364	L365	F366	T369	E 277	L378	N379	5380 5380	R383	S384	P385	1387 1387	L388	S389	L390	1392 1392	D393	D394	1.395 1.396	K397	K398	(1399 1700	K401		0406 E407		K414	1 1 0	L418 F419	R420	F421 M422	0423	E424	K425	V427	F428		1435 1 436	L430 A437	R438	R439	L440 L441		V446 S447
E451	1455	1458	K459	T460 E464	C462	G463	C464 0465	F466	T467	S468	E471		F474	MA 77	8478 S478	1479	S480	V496	004	V501	D502		R506	V507	T509	T510	G511 ve 10	V512 V513	P514	T515	P520	K521	C522 ME22	1524	P525	P526		TOCH	A541	K542	R546	Q547	L548
H552 H553 M554	G555	8556 4557	D558	L559 MEEO	A561	T562	TVR	GLY	PRO	VAL	LYS	GLU	ASP	GLY	GLU	VAL	GLY	CI V	GLY	ALA	GLN	THR	GLY	SER	T587		1591 1500	L592 0593	V594	8595 TEOG	1 33 0 F 59 7	<mark>0598</mark>	T COD		F605	N606	E COO	E009 K610	Y611	T612 E612	F013 E614	-	<mark>զ617</mark> զ618
E619 T620 D621	I622	P623 F624	R625	E626 1 607	V628	R629	DERO	S633	L634	A635	6637	K638	P639	T640	4041 R642	V643	L644	1645 K646	E647	P648	TGE2	E654	NG55	TEEO	600 I	Q664	F665	L669	H670	R671 W673	2104	K680	ປ681 ຕິເອີ	E683	-	E687	10000 10000	VOCA	R692	Q693	V695		K7 00 H7 01
E702 I703	A706	1707 V708	R709	1710 M711	K712	S713	R715 K715	K716	M717	1	L/22 V723	A724	E725	V726	R733	F734	L735	P/36	I741	K742	1 7/8	1749	E750	R751 E7E2	Y753	L754	176 A	1 / 0 4	A768														

• Molecule 3: Cullin-3















4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.590	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bond	angles
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.39	0/4558	0.49	0/6191
1	В	0.40	0/4548	0.50	0/6172
1	G	0.43	0/4521	0.51	0/6146
1	J	0.40	0/4569	0.48	0/6201
2	D	0.59	0/715	0.62	0/973
2	Ε	0.57	0/759	0.61	0/1029
2	Κ	0.55	0/759	0.61	0/1029
2	L	0.55	0/759	0.61	0/1029
3	С	0.43	0/5840	0.52	0/7853
3	F	0.46	0/5728	0.53	0/7706
3	Н	0.41	0/5806	0.52	0/7810
3	Ι	0.46	0/5802	0.54	0/7804
All	All	0.44	0/44364	0.52	0/59943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4455	18	4288	138	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	4446	18	4306	169	0
1	G	4420	18	4240	141	0
1	J	4464	18	4343	139	0
2	D	695	0	608	42	0
2	Е	737	0	686	57	0
2	Κ	737	0	686	54	0
2	L	737	0	686	58	0
3	С	5753	0	5709	193	0
3	F	5651	0	5542	190	0
3	Н	5719	0	5634	216	0
3	Ι	5722	0	5664	182	0
4	D	3	0	0	0	0
4	Е	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
All	All	43548	72	42392	1479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:47:MET:CE	1:J:21:LEU:HD22	1.45	1.44
2:K:24:VAL:C	2:K:25:LYS:HE2	1.43	1.38
2:D:24:VAL:C	2:D:25:LYS:HE2	1.43	1.38
2:L:24:VAL:C	2:L:25:LYS:HE2	1.43	1.35
2:E:24:VAL:C	2:E:25:LYS:HE2	1.43	1.35
3:I:665:PHE:HD1	3:I:665:PHE:O	1.07	1.31
3:F:665:PHE:HD1	3:F:665:PHE:O	1.07	1.29
3:H:665:PHE:HD1	3:H:665:PHE:O	1.07	1.29
3:C:730:LEU:HD13	3:C:733:ARG:NH2	1.43	1.29
3:C:665:PHE:HD1	3:C:665:PHE:O	1.07	1.27
3:I:665:PHE:O	3:I:665:PHE:CD1	1.89	1.25
3:C:665:PHE:O	3:C:665:PHE:CD1	1.89	1.25
3:F:665:PHE:O	3:F:665:PHE:CD1	1.89	1.25
3:H:665:PHE:O	3:H:665:PHE:CD1	1.89	1.25
2:E:97:ASP:OD2	2:E:99:ARG:HG2	1.37	1.21
1:B:160:PHE:CE2	1:B:169:PHE:CE1	2.30	1.20
2:K:25:LYS:HE2	2:K:25:LYS:N	1.58	1.18
2:L:25:LYS:HE2	2:L:25:LYS:N	1.58	1.16



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:25:LYS:HE2	2:E:25:LYS:N	1.58	1.15
2:D:25:LYS:HE2	2:D:25:LYS:N	1.58	1.15
3:F:626:GLU:HA	3:F:629:ARG:HD2	1.25	1.13
3:I:626:GLU:HA	3:I:629:ARG:HD2	1.25	1.13
3:H:638:LYS:HD3	3:H:639:PRO:HD2	1.30	1.12
3:I:638:LYS:HD3	3:I:639:PRO:HD2	1.29	1.12
3:F:638:LYS:HD3	3:F:639:PRO:HD2	1.29	1.11
1:G:47:MET:HE2	1:J:21:LEU:CD2	1.80	1.10
3:C:638:LYS:HD3	3:C:639:PRO:HD2	1.29	1.09
3:I:455:ILE:HG22	3:I:470:LEU:HD21	1.34	1.08
3:H:346:LEU:HA	3:H:418:LEU:HD12	1.34	1.07
3:H:455:ILE:HG22	3:H:470:LEU:HD21	1.34	1.06
3:C:730:LEU:CD1	3:C:733:ARG:NH2	2.20	1.05
1:G:47:MET:HG2	1:J:21:LEU:CD2	1.87	1.04
3:H:470:LEU:HD11	3:H:474:PHE:CE2	1.93	1.04
3:I:470:LEU:HD11	3:I:474:PHE:CE2	1.93	1.03
1:G:47:MET:SD	1:J:21:LEU:HD22	1.97	1.03
2:K:28:ASN:OD1	2:K:28:ASN:O	1.76	1.02
1:G:47:MET:HG2	1:J:21:LEU:HD21	1.42	1.02
1:G:233:TRP:CH2	1:G:245:VAL:HA	1.95	1.02
1:B:233:TRP:CH2	1:B:245:VAL:HA	1.95	1.02
2:L:28:ASN:OD1	2:L:28:ASN:O	1.76	1.02
2:E:28:ASN:OD1	2:E:28:ASN:O	1.76	1.01
2:D:28:ASN:OD1	2:D:28:ASN:O	1.76	1.01
3:F:441:LEU:HB3	3:F:554:MET:SD	2.01	1.00
1:J:233:TRP:CH2	1:J:245:VAL:HA	1.95	1.00
3:H:560:ASN:HB2	2:K:25:LYS:HG2	1.43	1.00
3:I:560:ASN:HB2	2:L:25:LYS:HG2	1.43	1.00
2:D:25:LYS:HG2	3:F:560:ASN:HB2	1.43	0.99
1:B:233:TRP:HH2	1:B:245:VAL:HA	1.26	0.99
1:J:233:TRP:HH2	1:J:245:VAL:HA	1.26	0.99
1:G:379:GLU:HG3	1:G:379:GLU:O	1.63	0.99
1:G:233:TRP:HH2	1:G:245:VAL:HA	1.26	0.98
1:G:47:MET:HE2	1:J:21:LEU:HD22	1.01	0.98
1:B:233:TRP:HH2	1:B:245:VAL:CA	1.76	0.98
3:C:560:ASN:HB2	2:E:25:LYS:HG2	1.43	0.98
2:L:24:VAL:C	2:L:25:LYS:CE	2.32	0.98
1:J:233:TRP:HH2	1:J:245:VAL:CA	1.76	0.97
2:D:24:VAL:C	2:D:25:LYS:CE	2.32	0.97
1:B:379:GLU:HG3	1:B:379:GLU:O	1.63	0.97
1:G:233:TRP:HH2	1:G:245:VAL:CA	1.76	0.97



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:24:VAL:C	2:K:25:LYS:CE	2.32	0.97
1:J:379:GLU:O	1:J:379:GLU:HG3	1.63	0.96
2:E:24:VAL:C	2:E:25:LYS:CE	2.32	0.96
3:H:248:VAL:HG22	3:H:256:THR:HG23	1.46	0.96
3:I:263:VAL:HG22	3:I:267:GLU:OE2	1.66	0.96
1:A:190:LYS:HB2	1:A:192:GLU:OE2	1.65	0.96
1:B:65:SER:HA	1:B:68:LYS:NZ	1.81	0.96
1:B:160:PHE:CE2	1:B:169:PHE:CZ	2.53	0.96
3:I:524:ILE:HG12	3:I:525:PRO:HD2	1.46	0.96
2:L:23:GLU:O	2:L:25:LYS:HE3	1.65	0.96
1:G:47:MET:CE	1:J:21:LEU:CD2	2.40	0.95
2:E:23:GLU:O	2:E:25:LYS:HE3	1.65	0.95
1:J:233:TRP:CH2	1:J:245:VAL:HG22	2.02	0.95
3:C:451:GLU:HB3	3:C:474:PHE:CZ	2.02	0.95
3:F:263:VAL:HG22	3:F:267:GLU:OE2	1.65	0.95
2:K:23:GLU:O	2:K:25:LYS:HE3	1.65	0.95
3:C:263:VAL:HG22	3:C:267:GLU:OE2	1.66	0.95
1:B:65:SER:CA	1:B:68:LYS:HZ1	1.78	0.95
1:B:190:LYS:HB2	1:B:192:GLU:OE2	1.65	0.95
3:F:248:VAL:HG22	3:F:256:THR:HG23	1.46	0.95
2:D:23:GLU:O	2:D:25:LYS:HE3	1.65	0.95
1:B:233:TRP:CH2	1:B:245:VAL:HG22	2.02	0.94
1:A:379:GLU:O	1:A:379:GLU:HG3	1.63	0.94
1:G:110:PHE:O	3:I:125:TYR:CE1	2.20	0.94
3:H:263:VAL:HG22	3:H:267:GLU:OE2	1.66	0.94
3:C:248:VAL:HG22	3:C:256:THR:HG23	1.46	0.94
1:G:233:TRP:CH2	1:G:245:VAL:HG22	2.02	0.93
3:C:730:LEU:HD13	3:C:733:ARG:CZ	1.97	0.92
1:A:370:ARG:HG2	1:A:389:SER:HA	1.51	0.91
3:H:225:LEU:HD11	3:H:275:THR:HG21	1.48	0.91
2:L:72:TRP:HB2	2:L:105:LYS:HB3	1.52	0.90
1:A:51:THR:HG21	1:B:17:LEU:CD1	2.01	0.90
3:I:455:ILE:HG22	3:I:470:LEU:CD2	2.01	0.90
3:I:524:ILE:HG12	3:I:525:PRO:CD	2.02	0.90
1:G:21:LEU:HD22	1:J:47:MET:HE2	1.53	0.90
2:K:72:TRP:HB2	2:K:105:LYS:HB3	1.52	0.90
1:G:151:SER:O	1:G:155:MET:HG2	1.71	0.89
3:F:735:LEU:HD13	3:F:736:PRO:HD2	1.54	0.89
1:G:181:LEU:HD22	1:G:219:GLN:HB3	1.54	0.89
3:C:506:ARG:HB2	2:E:30:VAL:HG22	1.55	0.89
1:A:151:SER:O	1:A:155:MET:HG2	1.71	0.89



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:G:47:MET:CG	1:J:21:LEU:CD2	2.50	0.89
3:H:455:ILE:HG22	3:H:470:LEU:CD2	2.01	0.89
1:B:151:SER:O	1:B:155:MET:HG2	1.71	0.89
2:E:72:TRP:HB2	2:E:105:LYS:HB3	1.52	0.89
2:D:72:TRP:HB2	2:D:105:LYS:HB3	1.53	0.89
3:H:506:ARG:HB2	2:K:30:VAL:HG22	1.55	0.88
2:D:30:VAL:HG22	3:F:506:ARG:HB2	1.55	0.88
1:B:65:SER:HA	1:B:68:LYS:HZ1	1.38	0.87
3:H:735:LEU:HD13	3:H:736:PRO:HD2	1.54	0.87
1:B:233:TRP:NE1	1:B:237:LEU:HB3	1.89	0.87
3:I:506:ARG:HB2	2:L:30:VAL:HG22	1.55	0.87
2:E:97:ASP:OD2	2:E:99:ARG:CG	2.22	0.87
1:J:233:TRP:NE1	1:J:237:LEU:HB3	1.90	0.86
1:G:233:TRP:NE1	1:G:237:LEU:HB3	1.89	0.86
3:H:346:LEU:HD13	3:H:418:LEU:HB2	1.57	0.86
1:B:160:PHE:CE2	1:B:169:PHE:CD1	2.63	0.86
3:C:730:LEU:HD13	3:C:733:ARG:HH22	1.35	0.86
1:J:161:THR:HB	1:J:188:VAL:HG13	1.59	0.85
1:B:65:SER:CA	1:B:68:LYS:NZ	2.37	0.85
3:C:413:ASP:HA	3:C:457:LYS:HE2	1.58	0.85
1:A:161:THR:HB	1:A:188:VAL:HG13	1.59	0.85
3:I:198:ARG:HH21	3:I:202:GLU:HG3	1.40	0.85
1:B:160:PHE:CZ	1:B:169:PHE:CZ	2.65	0.84
3:H:346:LEU:HD11	3:H:414:LYS:O	1.75	0.84
1:B:161:THR:HB	1:B:188:VAL:HG13	1.59	0.84
3:C:248:VAL:HG22	3:C:256:THR:CG2	2.08	0.84
3:C:669:LEU:HG	3:C:671:ARG:H	1.43	0.83
3:F:669:LEU:HG	3:F:671:ARG:H	1.43	0.83
3:F:248:VAL:HG22	3:F:256:THR:CG2	2.08	0.83
3:I:127:ASP:O	3:I:131:VAL:HG22	1.79	0.83
2:K:41:ASN:HD21	2:K:46:ARG:CD	1.92	0.83
3:C:751:ARG:NH2	3:C:753:TYR:HD1	1.76	0.83
1:A:24:PHE:HZ	1:B:57:ARG:HH22	1.26	0.82
3:I:669:LEU:HG	3:I:671:ARG:H	1.43	0.82
3:C:127:ASP:O	3:C:131:VAL:HG22	1.79	0.82
3:H:248:VAL:HG22	3:H:256:THR:CG2	2.08	0.82
3:H:669:LEU:HG	3:H:671:ARG:H	1.42	0.82
2:L:41:ASN:HD21	2:L:46:ARG:CD	1.92	0.82
2:E:41:ASN:HD21	2:E:46:ARG:CD	1.92	0.81
3:H:346:LEU:HB2	3:H:418:LEU:HD13	1.63	0.81
1:J:190:LYS:HG3	1:J:193:THR:HG22	1.61	0.81



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:H:127:ASP:O	3:H:131:VAL:HG22	1.79	0.81
3:H:346:LEU:CA	3:H:418:LEU:HD12	2.11	0.81
3:F:503:LEU:HD21	3:F:531:ALA:HB1	1.62	0.80
1:J:397:ARG:HD2	1:J:417:CYS:HA	1.63	0.80
1:B:262:GLY:O	1:B:265:LYS:HG2	1.82	0.80
1:J:262:GLY:O	1:J:265:LYS:HG2	1.82	0.80
3:H:346:LEU:HA	3:H:418:LEU:CD1	2.10	0.80
1:A:262:GLY:O	1:A:265:LYS:HG2	1.82	0.79
1:B:64:LEU:O	1:B:68:LYS:CE	2.30	0.79
1:B:202:LEU:HD22	1:B:213:LEU:HA	1.65	0.79
1:B:160:PHE:HE2	1:B:169:PHE:CE1	1.95	0.79
1:G:262:GLY:O	1:G:265:LYS:HG2	1.82	0.79
3:H:225:LEU:HD11	3:H:275:THR:CG2	2.10	0.79
1:A:17:LEU:CD1	1:B:51:THR:HG21	2.12	0.78
3:C:526:PRO:HA	3:C:529:ARG:HB2	1.65	0.78
1:A:181:LEU:HD22	1:A:219:GLN:HB3	1.65	0.78
1:B:160:PHE:HE2	1:B:169:PHE:CD1	2.02	0.78
3:H:346:LEU:CA	3:H:418:LEU:CD1	2.61	0.78
1:G:390:VAL:HG12	1:G:393:GLU:HG3	1.66	0.78
1:J:397:ARG:HG3	1:J:415:LEU:O	1.84	0.78
3:H:526:PRO:HA	3:H:529:ARG:HB2	1.65	0.77
1:G:47:MET:SD	1:J:21:LEU:CD2	2.71	0.77
3:F:541:ALA:HB2	3:H:501:VAL:O	1.84	0.77
3:C:751:ARG:HH21	3:C:753:TYR:HD1	1.33	0.77
3:F:440:LEU:HB2	3:F:513:TRP:CZ3	2.19	0.77
1:B:390:VAL:HG12	1:B:393:GLU:HG3	1.66	0.76
3:C:451:GLU:CB	3:C:474:PHE:CZ	2.67	0.76
1:A:51:THR:HG21	1:B:17:LEU:HD11	1.67	0.76
1:G:110:PHE:O	3:I:125:TYR:HE1	1.68	0.76
3:F:225:LEU:HB2	3:F:272:HIS:CE1	2.20	0.76
1:J:397:ARG:HD2	1:J:416:PRO:O	1.86	0.76
2:E:23:GLU:HB3	2:E:25:LYS:HZ1	1.49	0.75
3:F:120:ARG:HG3	3:F:140:TYR:HB2	1.68	0.75
3:H:458:LEU:HB3	3:H:467:THR:HG22	1.69	0.75
3:I:437:ALA:HA	3:I:513:TRP:HZ3	1.51	0.75
3:F:754:LEU:HD11	3:F:764:TYR:HB3	1.68	0.75
1:G:58:ALA:HB1	3:I:121:ASP:HB3	1.69	0.75
2:D:28:ASN:O	2:D:28:ASN:CG	2.25	0.75
3:F:440:LEU:HB2	3:F:513:TRP:HZ3	1.51	0.75
2:K:46:ARG:CZ	2:K:46:ARG:O	2.35	0.74
3:I:509:THR:HB	3:I:512:TYR:HD2	1.51	0.74



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:480:SER:HB2	3:C:506:ARG:HE	1.52	0.74
3:H:124:MET:HA	3:H:127:ASP:HB2	1.70	0.74
2:L:46:ARG:O	2:L:46:ARG:CZ	2.35	0.74
3:F:509:THR:HB	3:F:512:TYR:HD2	1.53	0.74
3:C:124:MET:HA	3:C:127:ASP:HB2	1.70	0.74
3:H:480:SER:HB2	3:H:506:ARG:HE	1.52	0.74
1:J:397:ARG:HB2	1:J:415:LEU:HB2	1.69	0.74
3:I:124:MET:HA	3:I:127:ASP:HB2	1.70	0.74
3:C:393:ASP:HA	3:C:439:ARG:HH21	1.52	0.74
3:H:120:ARG:HG3	3:H:140:TYR:HB2	1.68	0.74
3:C:416:MET:SD	3:C:457:LYS:HE3	2.28	0.74
2:E:46:ARG:CZ	2:E:46:ARG:O	2.35	0.74
1:A:47:MET:HE1	1:B:21:LEU:HD22	1.68	0.74
2:K:28:ASN:O	2:K:28:ASN:CG	2.25	0.74
3:C:451:GLU:HG2	3:C:474:PHE:HZ	1.53	0.74
3:I:470:LEU:HD11	3:I:474:PHE:HE2	1.51	0.74
3:I:120:ARG:HG3	3:I:140:TYR:HB2	1.68	0.73
1:J:397:ARG:HD2	1:J:417:CYS:CA	2.17	0.73
3:I:458:LEU:HB3	3:I:467:THR:HG22	1.69	0.73
1:A:181:LEU:HD21	1:A:220:ILE:HD13	1.70	0.73
2:E:28:ASN:O	2:E:28:ASN:CG	2.25	0.73
3:F:124:MET:HA	3:F:127:ASP:HB2	1.70	0.73
3:C:120:ARG:HG3	3:C:140:TYR:HB2	1.68	0.72
2:L:41:ASN:HD21	2:L:46:ARG:HD3	1.54	0.72
1:J:228:VAL:O	1:J:228:VAL:HG22	1.87	0.72
3:H:342:ILE:HG13	3:H:388:LEU:HA	1.71	0.72
3:C:245:ILE:HA	3:C:248:VAL:HG12	1.72	0.72
2:K:41:ASN:HD21	2:K:46:ARG:HD3	1.54	0.72
3:I:480:SER:HB2	3:I:506:ARG:HE	1.52	0.72
1:G:202:LEU:HD22	1:G:213:LEU:HA	1.71	0.72
1:G:273:GLU:HA	1:G:283:TYR:HB3	1.72	0.72
2:D:23:GLU:HB3	2:D:25:LYS:HZ1	1.55	0.72
3:H:470:LEU:HD11	3:H:474:PHE:HE2	1.51	0.72
3:F:245:ILE:HA	3:F:248:VAL:HG12	1.72	0.71
3:H:346:LEU:CD1	3:H:418:LEU:HB2	2.19	0.71
1:J:221:ARG:HA	1:J:255:LYS:HE2	1.72	0.71
1:A:21:LEU:HD22	1:B:47:MET:HE2	1.72	0.71
3:C:638:LYS:HD3	3:C:639:PRO:CD	2.16	0.71
2:E:41:ASN:HD21	2:E:46:ARG:HD3	1.54	0.71
1:G:233:TRP:CD1	1:G:237:LEU:HB3	2.26	0.70
2:D:24:VAL:O	2:D:25:LYS:HE2	1.91	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:24:VAL:O	2:L:25:LYS:HE2	1.91	0.70
1:B:233:TRP:CH2	1:B:245:VAL:CG2	2.74	0.70
1:B:65:SER:C	1:B:68:LYS:NZ	2.44	0.70
1:J:233:TRP:CH2	1:J:245:VAL:CG2	2.74	0.70
3:H:389:SER:HB2	3:H:431:TYR:HB3	1.73	0.70
1:B:233:TRP:CD1	1:B:237:LEU:HB3	2.26	0.70
3:I:638:LYS:HD3	3:I:639:PRO:CD	2.16	0.70
2:E:24:VAL:O	2:E:25:LYS:HE2	1.91	0.70
3:H:245:ILE:HA	3:H:248:VAL:HG12	1.72	0.70
3:F:638:LYS:HD3	3:F:639:PRO:CD	2.16	0.69
1:B:379:GLU:O	1:B:379:GLU:CG	2.40	0.69
1:G:47:MET:CG	1:J:21:LEU:HD22	2.20	0.69
1:J:233:TRP:CD1	1:J:237:LEU:HB3	2.26	0.69
3:H:638:LYS:HD3	3:H:639:PRO:CD	2.16	0.69
2:L:23:GLU:HB3	2:L:25:LYS:HZ1	1.58	0.69
3:H:735:LEU:CD1	3:H:736:PRO:HD2	2.22	0.69
3:F:166:LEU:HD22	3:F:212:MET:HG3	1.73	0.69
3:F:735:LEU:CD1	3:F:736:PRO:HD2	2.22	0.69
3:H:123:LEU:HB3	3:H:139:VAL:HG11	1.75	0.69
3:C:198:ARG:HH21	3:C:202:GLU:HG3	1.57	0.69
3:I:425:LYS:NZ	3:I:462:CYS:SG	2.64	0.69
3:C:123:LEU:HB3	3:C:139:VAL:HG11	1.75	0.69
2:K:47:ASN:HD21	2:K:54:ILE:HG23	1.58	0.69
1:A:17:LEU:HD11	1:B:51:THR:HG21	1.75	0.68
3:C:751:ARG:NH2	3:C:753:TYR:CD1	2.59	0.68
3:I:470:LEU:HD12	3:I:470:LEU:O	1.94	0.68
1:A:47:MET:CE	1:B:21:LEU:HD22	2.24	0.68
1:G:233:TRP:CH2	1:G:245:VAL:CG2	2.74	0.68
2:K:23:GLU:HB3	2:K:25:LYS:HZ1	1.59	0.68
2:K:24:VAL:O	2:K:25:LYS:HE2	1.91	0.68
3:I:123:LEU:HB3	3:I:139:VAL:HG11	1.75	0.68
2:L:28:ASN:O	2:L:28:ASN:CG	2.25	0.68
3:H:470:LEU:HD12	3:H:470:LEU:O	1.94	0.68
2:L:47:ASN:HD21	2:L:54:ILE:HG23	1.58	0.68
1:G:91:THR:HG23	1:G:93:ASN:H	1.59	0.67
1:B:233:TRP:CH2	1:B:245:VAL:CA	2.64	0.67
1:G:220:ILE:HG23	1:G:224:ALA:HB2	1.76	0.67
1:B:91:THR:HG23	1:B:93:ASN:H	1.59	0.67
3:C:730:LEU:CD1	3:C:733:ARG:HH22	1.97	0.67
2:E:47:ASN:HD21	2:E:54:ILE:HG23	1.58	0.67
3:F:123:LEU:HB3	3:F:139:VAL:HG11	1.75	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:707:ILE:HB	3:C:726:VAL:HG21	1.76	0.67
1:G:378:CYS:HB2	1:G:426:VAL:HG21	1.77	0.67
1:A:379:GLU:O	1:A:379:GLU:CG	2.40	0.67
2:K:23:GLU:HB3	2:K:25:LYS:NZ	2.10	0.67
1:B:378:CYS:HB2	1:B:426:VAL:HG21	1.77	0.67
2:D:23:GLU:HB3	2:D:25:LYS:NZ	2.10	0.67
2:E:23:GLU:HB3	2:E:25:LYS:NZ	2.10	0.67
3:I:446:VAL:HG23	3:I:447:SER:N	2.10	0.66
3:H:425:LYS:NZ	3:H:462:CYS:SG	2.64	0.66
2:L:23:GLU:HB3	2:L:25:LYS:NZ	2.10	0.66
1:A:19:GLU:OE2	1:B:8:GLN:NE2	2.28	0.66
1:J:378:CYS:HB2	1:J:426:VAL:HG21	1.77	0.66
1:J:91:THR:HG23	1:J:93:ASN:H	1.59	0.66
3:F:455:ILE:HD12	3:F:471:GLU:HG2	1.78	0.66
2:L:25:LYS:N	2:L:25:LYS:CE	2.50	0.66
3:I:90:ARG:NH2	3:I:150:GLN:OE1	2.29	0.66
1:G:190:LYS:HG3	1:G:193:THR:HG22	1.78	0.66
3:F:426:ASP:HB3	3:F:734:PHE:CD2	2.30	0.66
3:H:446:VAL:HG23	3:H:447:SER:N	2.10	0.66
1:B:65:SER:O	1:B:68:LYS:NZ	2.29	0.66
3:C:446:VAL:HG23	3:C:447:SER:N	2.10	0.65
3:C:451:GLU:CG	3:C:474:PHE:HZ	2.09	0.65
1:G:397:ARG:HB2	1:G:415:LEU:HB2	1.78	0.65
3:F:437:ALA:CB	3:F:514:PRO:CG	2.74	0.65
1:A:200:LEU:HA	1:A:203:GLU:HB2	1.78	0.65
2:L:72:TRP:HB2	2:L:105:LYS:CB	2.25	0.65
1:A:378:CYS:HB2	1:A:426:VAL:HG21	1.77	0.65
1:G:225:LEU:HD12	1:G:230:GLN:NE2	2.11	0.65
3:F:446:VAL:HG23	3:F:447:SER:N	2.10	0.65
2:K:72:TRP:HB2	2:K:105:LYS:CB	2.25	0.65
1:G:436:LEU:O	1:G:455:ARG:NH2	2.30	0.65
3:C:90:ARG:NH2	3:C:150:GLN:OE1	2.29	0.65
1:J:436:LEU:O	1:J:455:ARG:NH2	2.30	0.65
3:C:374:PHE:HB3	3:C:421:PHE:CG	2.31	0.65
1:A:436:LEU:O	1:A:455:ARG:NH2	2.30	0.64
3:F:90:ARG:NH2	3:F:150:GLN:OE1	2.29	0.64
1:B:436:LEU:O	1:B:455:ARG:NH2	2.30	0.64
3:H:90:ARG:NH2	3:H:150:GLN:OE1	2.29	0.64
3:I:509:THR:HB	3:I:512:TYR:CD2	2.33	0.64
3:I:180:ARG:HH22	3:I:250:HIS:HB3	1.63	0.64
3:I:546:ARG:HB2	2:L:33:TRP:HB2	1.77	0.64



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:I:559:LEU:HD22	3:I:602:LEU:HD23	1.80	0.64
3:I:508:LEU:HD13	3:I:513:TRP:CE2	2.32	0.64
3:C:556:SER:HA	3:C:595:SER:HA	1.80	0.64
1:B:64:LEU:O	1:B:68:LYS:NZ	2.31	0.63
2:D:25:LYS:N	2:D:25:LYS:CE	2.50	0.63
3:C:559:LEU:HD22	3:C:602:LEU:HD23	1.80	0.63
1:G:379:GLU:O	1:G:379:GLU:CG	2.40	0.63
3:I:198:ARG:O	3:I:202:GLU:HB3	1.99	0.63
3:C:451:GLU:CB	3:C:474:PHE:HZ	2.10	0.63
2:D:72:TRP:HB2	2:D:105:LYS:CB	2.25	0.63
3:F:440:LEU:HB3	3:F:513:TRP:HH2	1.64	0.63
3:I:522:CYS:HB3	3:I:622:ILE:HB	1.80	0.63
3:H:559:LEU:HD22	3:H:602:LEU:HD23	1.80	0.63
3:C:451:GLU:HB3	3:C:474:PHE:HZ	1.59	0.63
1:A:289:SER:HG	1:A:294:LYS:H	1.47	0.63
3:F:622:ILE:HG12	3:F:627:LEU:HD13	1.81	0.62
2:K:23:GLU:O	2:K:25:LYS:CE	2.46	0.62
1:B:64:LEU:C	1:B:68:LYS:HZ1	2.02	0.62
1:G:47:MET:CG	1:J:21:LEU:HD21	2.21	0.62
1:B:65:SER:HA	1:B:68:LYS:HZ3	1.61	0.62
1:J:289:SER:HG	1:J:294:LYS:H	1.48	0.62
3:F:556:SER:HA	3:F:595:SER:HA	1.80	0.62
3:H:346:LEU:CD1	3:H:414:LYS:O	2.48	0.62
2:L:41:ASN:ND2	2:L:46:ARG:CD	2.62	0.62
3:C:638:LYS:CG	3:C:642:ARG:HG2	2.30	0.62
3:F:559:LEU:HD22	3:F:602:LEU:HD23	1.80	0.62
3:H:638:LYS:CG	3:H:642:ARG:HG2	2.30	0.62
1:J:233:TRP:CH2	1:J:245:VAL:CA	2.64	0.62
3:H:173:ARG:HH12	3:H:213:SER:HA	1.63	0.62
3:H:198:ARG:HH21	3:H:202:GLU:HG3	1.64	0.62
3:H:556:SER:HA	3:H:595:SER:HA	1.80	0.62
3:H:682:GLY:O	3:H:683:GLU:CD	2.38	0.62
2:E:23:GLU:O	2:E:25:LYS:CE	2.46	0.62
3:C:682:GLY:O	3:C:683:GLU:CD	2.38	0.62
1:J:182:SER:HB3	1:J:219:GLN:HG3	1.82	0.62
3:F:248:VAL:CG2	3:F:256:THR:HG23	2.28	0.62
3:I:556:SER:HA	3:I:595:SER:HA	1.80	0.62
3:C:683:GLU:O	3:C:683:GLU:HG2	2.00	0.62
3:H:683:GLU:O	3:H:683:GLU:HG2	2.00	0.62
3:I:682:GLY:O	3:I:683:GLU:CD	2.38	0.62
1:A:273:GLU:HA	1:A:283:TYR:HB3	1.82	0.61



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:426:ASP:HB3	3:F:734:PHE:HD2	1.65	0.61
2:E:72:TRP:HB2	2:E:105:LYS:CB	2.25	0.61
3:F:458:LEU:HB3	3:F:467:THR:HB	1.83	0.61
3:I:634:LEU:HB3	3:I:644:LEU:HD23	1.82	0.61
3:C:248:VAL:CG2	3:C:256:THR:HG23	2.28	0.61
3:C:509:THR:HB	3:C:512:TYR:HD2	1.64	0.61
3:C:560:ASN:HB2	2:E:25:LYS:CG	2.27	0.61
3:F:682:GLY:O	3:F:683:GLU:CD	2.38	0.61
3:F:598:GLN:HG2	3:F:634:LEU:HG	1.83	0.61
3:F:683:GLU:O	3:F:683:GLU:HG2	2.00	0.61
3:H:509:THR:HB	3:H:512:TYR:HD1	1.64	0.61
1:A:24:PHE:HZ	1:B:57:ARG:NH2	1.98	0.61
1:A:55:TYR:CE1	3:C:58:TYR:CB	2.84	0.61
3:H:560:ASN:HB2	2:K:25:LYS:CG	2.27	0.61
2:K:41:ASN:ND2	2:K:46:ARG:CD	2.62	0.61
3:I:683:GLU:HG2	3:I:683:GLU:O	2.00	0.61
2:L:23:GLU:O	2:L:25:LYS:CE	2.46	0.61
1:B:273:GLU:HA	1:B:283:TYR:HB3	1.82	0.61
3:F:638:LYS:CG	3:F:642:ARG:HG2	2.30	0.61
1:G:231:ARG:H	1:G:231:ARG:HD2	1.66	0.61
3:H:424:GLU:OE2	3:H:735:LEU:HD23	2.01	0.61
3:I:638:LYS:CG	3:I:642:ARG:HG2	2.30	0.61
3:H:220:GLU:HA	3:H:223:LYS:HB2	1.83	0.61
2:L:23:GLU:C	2:L:25:LYS:HE3	2.22	0.61
2:D:23:GLU:O	2:D:25:LYS:CE	2.46	0.61
2:K:25:LYS:HE2	2:K:25:LYS:CA	2.31	0.61
1:A:127:LYS:HG3	1:A:127:LYS:O	2.01	0.60
1:B:231:ARG:H	1:B:231:ARG:HD2	1.66	0.60
3:I:598:GLN:HG2	3:I:634:LEU:HG	1.83	0.60
2:E:25:LYS:HE2	2:E:25:LYS:CA	2.31	0.60
1:J:127:LYS:O	1:J:127:LYS:HG3	2.02	0.60
2:L:25:LYS:HE2	2:L:25:LYS:CA	2.32	0.60
1:G:186:LEU:HD13	1:G:194:VAL:HG11	1.83	0.60
3:H:598:GLN:HG2	3:H:634:LEU:HG	1.83	0.60
3:I:509:THR:HG23	2:L:76:ASN:ND2	2.17	0.60
1:J:231:ARG:H	1:J:231:ARG:HD2	1.66	0.60
3:F:634:LEU:HB3	3:F:644:LEU:HD23	1.82	0.60
3:H:346:LEU:HD13	3:H:418:LEU:CB	2.31	0.60
2:K:23:GLU:C	2:K:25:LYS:HE3	2.22	0.60
1:J:399:VAL:HG13	1:J:415:LEU:HD21	1.82	0.60
3:H:634:LEU:HB3	3:H:644:LEU:HD23	1.82	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
3:C:634:LEU:HB3	3:C:644:LEU:HD23	1.82	0.60
3:F:204:ASP:O	3:F:208:PRO:HD2	2.01	0.60
3:F:440:LEU:CB	3:F:513:TRP:CH2	2.85	0.60
3:I:385:PRO:HB3	3:I:428:PHE:HB2	1.83	0.60
3:C:451:GLU:HG2	3:C:474:PHE:CZ	2.36	0.60
1:J:273:GLU:HA	1:J:283:TYR:HB3	1.83	0.60
3:I:153:ARG:HH21	3:I:200:VAL:HG13	1.66	0.60
3:H:508:LEU:HD13	3:H:513:TRP:CE2	2.36	0.60
3:C:598:GLN:HG2	3:C:634:LEU:HG	1.83	0.60
1:A:153:LYS:HE3	1:A:179:ASP:OD1	2.02	0.60
3:F:437:ALA:HB2	3:F:514:PRO:CD	2.31	0.60
3:H:356:LEU:HD12	3:H:360:PHE:HB2	1.84	0.60
3:I:622:ILE:HG12	3:I:627:LEU:HD13	1.84	0.60
3:C:451:GLU:HB3	3:C:474:PHE:CE2	2.37	0.60
1:B:153:LYS:HE3	1:B:179:ASP:OD1	2.02	0.59
1:G:127:LYS:O	1:G:127:LYS:HG3	2.01	0.59
1:J:153:LYS:HE3	1:J:179:ASP:OD1	2.02	0.59
2:D:23:GLU:C	2:D:25:LYS:HE3	2.22	0.59
2:K:24:VAL:O	2:K:25:LYS:CE	2.49	0.59
2:E:41:ASN:ND2	2:E:46:ARG:CD	2.62	0.59
1:B:397:ARG:HB2	1:B:415:LEU:HB2	1.84	0.59
3:I:626:GLU:CA	3:I:629:ARG:HD2	2.18	0.59
2:E:23:GLU:C	2:E:25:LYS:HE3	2.22	0.59
2:E:25:LYS:N	2:E:25:LYS:CE	2.50	0.59
3:F:339:VAL:HA	3:F:391:PHE:HB2	1.84	0.59
1:A:57:ARG:HH22	1:B:24:PHE:HZ	1.49	0.59
3:F:217:PHE:HB2	3:F:267:GLU:OE1	2.03	0.59
3:H:641:GLN:HA	3:H:641:GLN:OE1	2.02	0.59
3:C:282:SER:HA	3:C:286:HIS:HB3	1.85	0.59
1:G:535:CYS:SG	1:G:564:ARG:NH1	2.76	0.59
2:K:25:LYS:N	2:K:25:LYS:CE	2.50	0.59
3:C:102:LEU:HD11	3:C:182:ALA:HB1	1.85	0.59
3:C:414:LYS:O	3:C:418:LEU:HG	2.03	0.59
1:G:289:SER:HG	1:G:294:LYS:H	1.49	0.59
3:I:641:GLN:OE1	3:I:641:GLN:HA	2.02	0.59
1:A:382:ILE:HB	1:A:402:TYR:HB3	1.85	0.59
1:G:127:LYS:O	1:G:127:LYS:CG	2.51	0.59
3:H:525:PRO:HB2	3:H:528:PRO:HG2	1.83	0.59
3:I:768:ALA:HB1	2:L:89:LYS:HB3	1.85	0.59
1:G:153:LYS:HE3	1:G:179:ASP:OD1	2.02	0.59
3:H:337:ASN:ND2	3:H:340:ASP:OD1	2.35	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:I:102:LEU:HD11	3:I:182:ALA:HB1	1.85	0.59
1:B:233:TRP:HE1	1:B:237:LEU:HB3	1.68	0.58
3:H:473:MET:SD	3:H:512:TYR:HB3	2.43	0.58
3:I:207:ALA:HB3	3:I:208:PRO:HD3	1.85	0.58
3:C:356:LEU:HD12	3:C:360:PHE:HB2	1.84	0.58
1:J:397:ARG:HD2	1:J:416:PRO:C	2.23	0.58
3:F:446:VAL:CG2	3:F:447:SER:N	2.67	0.58
3:H:282:SER:HA	3:H:286:HIS:HB3	1.85	0.58
3:F:626:GLU:CA	3:F:629:ARG:HD2	2.18	0.58
3:H:389:SER:HB2	3:H:431:TYR:CB	2.34	0.58
3:H:446:VAL:CG2	3:H:447:SER:N	2.66	0.58
3:F:102:LEU:HD11	3:F:182:ALA:HB1	1.85	0.58
1:A:186:LEU:HD13	1:A:194:VAL:HG11	1.85	0.58
1:A:207:GLU:HG3	1:A:238:PRO:HG3	1.85	0.58
1:B:127:LYS:O	1:B:127:LYS:HG3	2.01	0.58
1:B:535:CYS:SG	1:B:564:ARG:NH1	2.76	0.58
1:J:535:CYS:SG	1:J:564:ARG:NH1	2.76	0.58
3:F:43:GLU:OE2	3:F:48:ASN:ND2	2.32	0.58
3:F:706:ALA:HA	3:F:709:ARG:HH21	1.68	0.58
3:I:560:ASN:HB2	2:L:25:LYS:CG	2.27	0.58
2:E:24:VAL:O	2:E:25:LYS:CE	2.49	0.58
2:D:25:LYS:CG	3:F:560:ASN:HB2	2.27	0.58
3:H:238:GLU:O	3:H:242:ASN:ND2	2.32	0.58
3:I:282:SER:HA	3:I:286:HIS:HB3	1.85	0.58
1:B:186:LEU:HD13	1:B:194:VAL:HG11	1.86	0.58
1:B:382:ILE:HB	1:B:402:TYR:HB3	1.85	0.58
1:J:127:LYS:O	1:J:127:LYS:CG	2.51	0.58
1:B:289:SER:HG	1:B:294:LYS:H	1.51	0.58
3:F:349:LYS:HE2	3:F:421:PHE:HE2	1.69	0.58
3:H:102:LEU:HD11	3:H:182:ALA:HB1	1.85	0.58
3:I:238:GLU:O	3:I:242:ASN:ND2	2.32	0.58
1:A:127:LYS:O	1:A:127:LYS:CG	2.51	0.58
1:A:535:CYS:SG	1:A:564:ARG:NH1	2.76	0.58
1:B:459:ARG:HB3	1:B:476:GLY:HA3	1.86	0.58
3:I:446:VAL:CG2	3:I:447:SER:N	2.67	0.58
1:B:127:LYS:O	1:B:127:LYS:CG	2.51	0.58
1:J:233:TRP:HE1	1:J:237:LEU:HB3	1.69	0.58
3:F:700:LYS:O	3:F:703:ILE:HG12	2.04	0.58
2:L:35:TRP:HD1	2:L:75:CYS:O	1.87	0.58
1:A:55:TYR:HE1	3:C:58:TYR:CB	2.17	0.57
1:G:459:ARG:HB3	1:G:476:GLY:HA3	1.86	0.57



	o uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:441:LEU:HD21	3:F:508:LEU:CD1	2.34	0.57
2:L:46:ARG:O	2:L:46:ARG:NE	2.37	0.57
3:C:641:GLN:HA	3:C:641:GLN:OE1	2.02	0.57
2:D:77:HIS:CD2	2:D:96:LEU:CD1	2.87	0.57
2:K:46:ARG:O	2:K:46:ARG:NE	2.37	0.57
3:C:446:VAL:CG2	3:C:447:SER:N	2.66	0.57
1:A:19:GLU:CD	1:B:8:GLN:HE21	2.06	0.57
2:D:35:TRP:HD1	2:D:75:CYS:O	1.86	0.57
2:L:38:VAL:HG12	2:L:41:ASN:N	2.18	0.57
3:C:509:THR:HG23	2:E:76:ASN:ND2	2.19	0.57
2:E:38:VAL:HG12	2:E:41:ASN:N	2.18	0.57
1:G:93:ASN:HD21	1:J:9:ILE:HG23	1.70	0.57
1:G:233:TRP:CZ3	1:G:245:VAL:HA	2.38	0.57
2:D:25:LYS:HE2	2:D:25:LYS:CA	2.32	0.57
2:L:24:VAL:O	2:L:25:LYS:CE	2.49	0.57
1:G:233:TRP:HE1	1:G:237:LEU:HB3	1.68	0.57
3:F:282:SER:HA	3:F:286:HIS:HB3	1.85	0.57
3:F:509:THR:HB	3:F:512:TYR:CD2	2.36	0.57
2:K:35:TRP:HD1	2:K:75:CYS:O	1.86	0.57
1:A:91:THR:HG23	1:A:93:ASN:H	1.69	0.57
3:F:440:LEU:HB3	3:F:513:TRP:CH2	2.39	0.57
3:H:346:LEU:CB	3:H:418:LEU:HD13	2.32	0.57
2:K:38:VAL:HG12	2:K:41:ASN:N	2.18	0.57
3:C:455:ILE:C	3:C:457:LYS:N	2.54	0.57
1:A:476:GLY:O	1:A:496:SER:N	2.38	0.57
3:F:337:ASN:HB3	3:F:340:ASP:HB2	1.85	0.57
3:F:641:GLN:HA	3:F:641:GLN:OE1	2.02	0.57
3:C:238:GLU:O	3:C:242:ASN:ND2	2.32	0.57
2:E:24:VAL:O	2:E:25:LYS:NZ	2.38	0.57
2:E:35:TRP:HD1	2:E:75:CYS:O	1.86	0.57
1:B:217:LEU:HG	1:B:225:LEU:HD11	1.86	0.57
3:F:446:VAL:CG2	3:F:447:SER:H	2.18	0.57
1:B:476:GLY:O	1:B:496:SER:N	2.38	0.57
3:H:245:ILE:HA	3:H:248:VAL:CG1	2.35	0.57
3:H:638:LYS:HG2	3:H:642:ARG:HG2	1.87	0.57
2:K:24:VAL:O	2:K:25:LYS:NZ	2.38	0.57
3:C:289:LYS:O	3:C:351:ARG:NH2	2.38	0.57
2:E:23:GLU:C	2:E:25:LYS:CE	2.73	0.57
2:L:23:GLU:C	2:L:25:LYS:CE	2.74	0.57
3:C:638:LYS:HG2	3:C:642:ARG:HG2	1.87	0.57
1:A:459:ARG:HB3	1:A:476:GLY:HA3	1.86	0.56



	li al pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:181:LEU:HD21	1:B:220:ILE:HD13	1.86	0.56
1:J:233:TRP:CZ3	1:J:245:VAL:HA	2.38	0.56
3:I:625:ARG:H	3:I:625:ARG:HH21	1.51	0.56
3:I:638:LYS:HG2	3:I:642:ARG:HG2	1.87	0.56
3:C:446:VAL:CG2	3:C:447:SER:H	2.18	0.56
1:J:379:GLU:O	1:J:379:GLU:CG	2.40	0.56
3:F:437:ALA:CB	3:F:514:PRO:HG3	2.35	0.56
1:B:525:VAL:HA	1:B:538:MET:HG2	1.88	0.56
1:J:476:GLY:O	1:J:496:SER:N	2.38	0.56
2:D:23:GLU:C	2:D:25:LYS:CE	2.74	0.56
3:F:638:LYS:HG2	3:F:642:ARG:HG2	1.87	0.56
3:H:289:LYS:O	3:H:351:ARG:NH2	2.38	0.56
3:I:612:THR:OG1	3:I:655:ASN:O	2.24	0.56
3:C:699:ARG:HE	3:C:734:PHE:HB2	1.70	0.56
1:G:286:VAL:HG11	1:G:573:TRP:HH2	1.71	0.56
2:D:24:VAL:O	2:D:25:LYS:CE	2.50	0.56
3:F:612:THR:OG1	3:F:655:ASN:O	2.24	0.56
3:H:383:ARG:HD3	3:H:387:TYR:CZ	2.40	0.56
3:C:557:ALA:HB3	3:C:594:VAL:HG23	1.88	0.56
2:E:46:ARG:O	2:E:46:ARG:NE	2.37	0.56
1:B:305:LEU:HD21	1:B:323:GLY:HA3	1.88	0.56
1:J:228:VAL:O	1:J:228:VAL:CG2	2.54	0.56
3:H:557:ALA:HB3	3:H:594:VAL:HG23	1.88	0.56
2:L:24:VAL:O	2:L:25:LYS:NZ	2.38	0.56
3:C:612:THR:OG1	3:C:655:ASN:O	2.24	0.56
1:G:525:VAL:HA	1:G:538:MET:HG2	1.88	0.56
1:J:166:GLN:HB2	1:J:169:PHE:HB3	1.88	0.56
2:D:24:VAL:O	2:D:25:LYS:NZ	2.38	0.56
1:A:234:PHE:O	1:A:237:LEU:HG	2.05	0.56
1:A:305:LEU:HD21	1:A:323:GLY:HA3	1.88	0.56
1:G:476:GLY:O	1:G:496:SER:N	2.38	0.56
1:J:459:ARG:HB3	1:J:476:GLY:HA3	1.86	0.56
3:H:612:THR:OG1	3:H:655:ASN:O	2.24	0.56
1:B:64:LEU:O	1:B:68:LYS:HE3	2.04	0.56
1:J:305:LEU:HD21	1:J:323:GLY:HA3	1.88	0.56
2:K:23:GLU:C	2:K:25:LYS:CE	2.74	0.56
3:C:245:ILE:HA	3:C:248:VAL:CG1	2.35	0.56
3:F:245:ILE:HA	3:F:248:VAL:CG1	2.35	0.56
3:F:682:GLY:O	3:F:683:GLU:CG	2.54	0.56
3:H:437:ALA:HA	3:H:513:TRP:HZ3	1.71	0.56
3:C:415:ALA:HA	3:C:418:LEU:HD12	1.87	0.56



	io de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:27:TRP:CZ2	2:E:29:ALA:HB2	2.40	0.56
2:D:76:ASN:ND2	3:F:509:THR:HG23	2.21	0.55
2:K:27:TRP:CZ2	2:K:29:ALA:HB2	2.40	0.55
2:L:27:TRP:CZ2	2:L:29:ALA:HB2	2.40	0.55
3:H:446:VAL:CG2	3:H:447:SER:H	2.18	0.55
3:C:144:LEU:HD12	3:C:193:LEU:HA	1.88	0.55
1:A:254:PRO:O	1:A:255:LYS:HG2	2.06	0.55
3:F:144:LEU:HD12	3:F:193:LEU:HA	1.88	0.55
3:H:473:MET:HG2	3:H:512:TYR:HB3	1.87	0.55
3:H:682:GLY:O	3:H:683:GLU:CG	2.54	0.55
3:I:446:VAL:CG2	3:I:447:SER:H	2.18	0.55
3:I:682:GLY:O	3:I:683:GLU:CG	2.54	0.55
2:L:47:ASN:HD21	2:L:54:ILE:CG2	2.18	0.55
3:C:129:VAL:O	3:C:133:GLN:NE2	2.34	0.55
1:B:286:VAL:HG11	1:B:573:TRP:HH2	1.71	0.55
1:J:198:ALA:O	1:J:202:LEU:HG	2.06	0.55
1:J:397:ARG:CD	1:J:416:PRO:O	2.55	0.55
3:I:559:LEU:CD2	3:I:602:LEU:HD23	2.36	0.55
3:C:525:PRO:HB2	3:C:528:PRO:HG2	1.87	0.55
3:C:682:GLY:O	3:C:683:GLU:CG	2.54	0.55
1:B:233:TRP:HH2	1:B:245:VAL:N	2.04	0.55
1:B:254:PRO:O	1:B:255:LYS:HG2	2.06	0.55
1:J:254:PRO:O	1:J:255:LYS:HG2	2.06	0.55
3:F:557:ALA:HB3	3:F:594:VAL:HG23	1.88	0.55
3:F:559:LEU:CD2	3:F:602:LEU:HD23	2.36	0.55
2:K:47:ASN:HD21	2:K:54:ILE:CG2	2.18	0.55
3:I:129:VAL:O	3:I:133:GLN:NE2	2.34	0.55
3:I:144:LEU:HD12	3:I:193:LEU:HA	1.88	0.55
1:B:233:TRP:CZ3	1:B:245:VAL:HA	2.38	0.55
1:J:286:VAL:HG11	1:J:573:TRP:HH2	1.71	0.55
2:K:38:VAL:HG12	2:K:41:ASN:H	1.72	0.55
1:B:195:ARG:HB2	1:B:224:ALA:HB1	1.89	0.55
3:H:710:ILE:HG21	3:H:729:GLN:HE22	1.71	0.55
1:G:233:TRP:HH2	1:G:245:VAL:N	2.04	0.55
1:J:233:TRP:HH2	1:J:245:VAL:N	2.04	0.55
2:D:27:TRP:CZ2	2:D:29:ALA:HB2	2.40	0.55
3:F:717:MET:HB3	3:F:722:LEU:HG	1.89	0.55
3:H:717:MET:HB3	3:H:722:LEU:HG	1.89	0.55
2:L:71:ALA:HB2	2:L:81:PHE:HA	1.88	0.55
3:C:717:MET:HB3	3:C:722:LEU:HG	1.89	0.55
1:J:207:GLU:HG3	1:J:238:PRO:HG3	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:H:314:CYS:HB3	3:H:369:THR:HG21	1.89	0.55
3:H:409:GLU:OE2	3:H:453:ASN:ND2	2.40	0.55
3:C:314:CYS:HB3	3:C:369:THR:HG21	1.89	0.55
1:A:53:SER:OG	1:A:111:LEU:O	2.25	0.55
1:G:305:LEU:HD21	1:G:323:GLY:HA3	1.88	0.55
3:H:559:LEU:CD2	3:H:602:LEU:HD23	2.36	0.55
3:I:314:CYS:HB3	3:I:369:THR:HG21	1.89	0.55
3:I:418:LEU:O	3:I:422:MET:HG3	2.06	0.55
3:C:559:LEU:CD2	3:C:602:LEU:HD23	2.36	0.55
1:J:525:VAL:HA	1:J:538:MET:HG2	1.88	0.54
1:G:555:ASP:HB3	1:G:558:LEU:HB2	1.90	0.54
3:F:342:ILE:HG13	3:F:388:LEU:HA	1.89	0.54
3:H:144:LEU:HD12	3:H:193:LEU:HA	1.88	0.54
3:C:338:PRO:HA	3:C:341:TYR:HD2	1.72	0.54
3:C:641:GLN:OE1	3:C:664:GLN:HB3	2.08	0.54
1:J:53:SER:OG	1:J:111:LEU:O	2.25	0.54
3:I:751:ARG:NH2	2:L:55:GLU:HB3	2.22	0.54
2:E:84:ILE:HG12	2:E:101:TRP:CE2	2.43	0.54
1:A:525:VAL:HA	1:A:538:MET:HG2	1.88	0.54
3:H:346:LEU:HD11	3:H:414:LYS:C	2.28	0.54
3:H:641:GLN:OE1	3:H:664:GLN:HB3	2.08	0.54
2:E:47:ASN:HD21	2:E:54:ILE:CG2	2.18	0.54
1:B:555:ASP:HB3	1:B:558:LEU:HB2	1.90	0.54
3:H:768:ALA:HB1	2:K:89:LYS:HB3	1.90	0.54
3:I:557:ALA:HB3	3:I:594:VAL:HG23	1.88	0.54
3:F:638:LYS:HG3	3:F:639:PRO:O	2.08	0.54
3:H:466:PHE:HA	3:H:469:LYS:HG2	1.89	0.54
1:B:160:PHE:HE2	1:B:169:PHE:CG	2.25	0.54
3:H:622:ILE:HG12	3:H:627:LEU:HD13	1.89	0.54
3:I:466:PHE:HA	3:I:469:LYS:HG2	1.89	0.54
1:B:365:PRO:O	1:B:409:TRP:NE1	2.41	0.54
1:J:370:ARG:HG2	1:J:389:SER:HA	1.90	0.54
3:I:225:LEU:HB3	3:I:272:HIS:CE1	2.43	0.54
3:H:638:LYS:HG3	3:H:639:PRO:O	2.08	0.54
3:I:638:LYS:HG3	3:I:639:PRO:O	2.08	0.54
3:I:641:GLN:OE1	3:I:664:GLN:HB3	2.08	0.54
2:L:38:VAL:HG12	2:L:41:ASN:H	1.72	0.54
1:A:51:THR:CG2	1:B:17:LEU:CD1	2.82	0.53
1:A:286:VAL:HG11	1:A:573:TRP:HH2	1.71	0.53
1:G:10:ASN:HB2	1:G:14:ALA:H	1.74	0.53
3:C:638:LYS:HG3	3:C:639:PRO:O	2.09	0.53



	h h c	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:J:365:PRO:O	1:J:409:TRP:NE1	2.41	0.53
3:F:153:ARG:HH21	3:F:200:VAL:HG13	1.74	0.53
1:G:161:THR:HB	1:G:188:VAL:HG13	1.90	0.53
2:D:93:VAL:HA	2:D:100:GLU:HA	1.91	0.53
3:F:440:LEU:CB	3:F:513:TRP:HH2	2.21	0.53
3:H:169:ILE:HD11	3:H:247:ARG:HD3	1.91	0.53
3:I:614:GLU:OE1	3:I:617:GLN:NE2	2.41	0.53
3:F:169:ILE:HD11	3:F:247:ARG:HD3	1.91	0.53
1:A:348:ASN:ND2	1:A:366:MET:O	2.42	0.53
1:G:370:ARG:HG2	1:G:389:SER:HA	1.90	0.53
3:F:625:ARG:H	3:F:625:ARG:HH21	1.55	0.53
2:L:41:ASN:ND2	2:L:46:ARG:HG2	2.24	0.53
1:G:365:PRO:O	1:G:409:TRP:NE1	2.41	0.53
3:F:614:GLU:OE1	3:F:617:GLN:NE2	2.41	0.53
3:H:393:ASP:HB2	3:H:435:HIS:NE2	2.24	0.53
3:I:166:LEU:HD11	3:I:208:PRO:HB3	1.90	0.53
3:C:614:GLU:OE1	3:C:617:GLN:NE2	2.41	0.53
2:E:41:ASN:ND2	2:E:46:ARG:HG2	2.24	0.53
2:D:77:HIS:CD2	2:D:96:LEU:HD12	2.44	0.53
1:A:13:TYR:OH	1:B:89:ALA:HA	2.08	0.53
3:F:641:GLN:OE1	3:F:664:GLN:HB3	2.08	0.53
3:C:506:ARG:O	2:E:31:ALA:N	2.35	0.53
1:A:555:ASP:HB3	1:A:558:LEU:HB2	1.90	0.53
1:B:431:ILE:HB	1:B:442:TYR:HB3	1.91	0.53
1:G:263:MET:SD	1:G:263:MET:N	2.82	0.53
1:J:414:PRO:O	1:J:449:TRP:NE1	2.42	0.53
3:F:116:MET:HA	3:F:119:ILE:HB	1.91	0.53
3:H:248:VAL:CG2	3:H:256:THR:HG23	2.27	0.53
2:E:38:VAL:HG12	2:E:41:ASN:H	1.72	0.53
1:B:548:LYS:NZ	1:B:549:TYR:O	2.42	0.52
3:H:346:LEU:N	3:H:418:LEU:CD1	2.71	0.52
3:H:506:ARG:O	2:K:31:ALA:N	2.34	0.52
3:I:606:ASN:HD21	2:L:22:PHE:HD2	1.57	0.52
3:C:626:GLU:HA	3:C:629:ARG:HH11	1.74	0.52
1:A:263:MET:SD	1:A:263:MET:N	2.83	0.52
1:A:365:PRO:O	1:A:409:TRP:NE1	2.41	0.52
1:J:548:LYS:NZ	1:J:549:TYR:O	2.42	0.52
1:J:555:ASP:HB3	1:J:558:LEU:HB2	1.90	0.52
3:H:190:LEU:HB3	3:H:201:TYR:HB2	1.90	0.52
3:I:116:MET:HA	3:I:119:ILE:HB	1.90	0.52
2:L:47:ASN:ND2	2:L:54:ILE:HG23	2.24	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:414:PRO:O	1:G:449:TRP:NE1	2.42	0.52
1:J:263:MET:SD	1:J:263:MET:N	2.83	0.52
3:H:116:MET:HA	3:H:119:ILE:HB	1.90	0.52
1:A:548:LYS:NZ	1:A:549:TYR:O	2.42	0.52
1:B:553:GLN:HB2	1:B:564:ARG:HB2	1.91	0.52
1:G:348:ASN:ND2	1:G:366:MET:O	2.42	0.52
2:D:22:PHE:HD2	3:F:606:ASN:HD21	1.57	0.52
2:D:33:TRP:HB2	3:F:546:ARG:HB2	1.92	0.52
3:H:441:LEU:HD21	3:H:508:LEU:HD11	1.91	0.52
2:K:41:ASN:ND2	2:K:46:ARG:HG2	2.24	0.52
3:C:509:THR:HB	3:C:512:TYR:CD2	2.44	0.52
1:J:228:VAL:HG23	1:J:231:ARG:HB2	1.91	0.52
3:H:606:ASN:HD21	2:K:22:PHE:HD1	1.57	0.52
3:H:614:GLU:OE1	3:H:617:GLN:NE2	2.41	0.52
3:H:708:VAL:HA	3:H:754:LEU:HD23	1.91	0.52
2:K:84:ILE:HG12	2:K:101:TRP:CE2	2.44	0.52
1:B:297:LYS:NZ	1:B:593:GLU:O	2.43	0.52
1:B:370:ARG:HG2	1:B:389:SER:HA	1.90	0.52
1:G:301:PRO:HG3	1:G:360:TRP:CE2	2.45	0.52
3:F:541:ALA:HB2	3:H:502:ASP:HA	1.91	0.52
3:H:700:LYS:O	3:H:703:ILE:HG12	2.09	0.52
3:C:116:MET:HA	3:C:119:ILE:HB	1.91	0.52
1:J:348:ASN:ND2	1:J:366:MET:O	2.42	0.52
3:F:522:CYS:HB2	3:F:622:ILE:HB	1.92	0.52
3:H:509:THR:HB	3:H:512:TYR:CD1	2.44	0.52
3:I:102:LEU:CD1	3:I:182:ALA:HB1	2.40	0.52
3:C:169:ILE:HD11	3:C:247:ARG:HD3	1.91	0.52
3:F:202:GLU:O	3:F:203:GLU:C	2.46	0.52
3:I:169:ILE:HD11	3:I:247:ARG:HD3	1.91	0.52
1:B:522:ASP:N	1:B:522:ASP:OD1	2.43	0.52
1:G:233:TRP:CH2	1:G:245:VAL:CA	2.65	0.52
3:C:102:LEU:CD1	3:C:182:ALA:HB1	2.40	0.52
1:B:348:ASN:ND2	1:B:366:MET:O	2.42	0.51
3:F:102:LEU:CD1	3:F:182:ALA:HB1	2.40	0.51
3:F:542:LYS:HA	3:H:488:ARG:CB	2.40	0.51
3:C:455:ILE:C	3:C:457:LYS:H	2.12	0.51
1:A:21:LEU:HD22	1:B:47:MET:CE	2.39	0.51
1:A:321:ALA:HB3	1:A:375:LEU:HD11	1.92	0.51
1:J:553:GLN:HB2	1:J:564:ARG:HB2	1.91	0.51
2:E:47:ASN:ND2	2:E:54:ILE:HG23	2.24	0.51
1:A:297:LYS:NZ	1:A:593:GLU:O	2.43	0.51



	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:B:263:MET:SD	1:B:263:MET:N	2.82	0.51
1:B:374:SER:OG	1:B:385:ILE:O	2.28	0.51
1:J:301:PRO:HG3	1:J:360:TRP:CE2	2.45	0.51
3:H:102:LEU:CD1	3:H:182:ALA:HB1	2.40	0.51
3:H:129:VAL:O	3:H:133:GLN:NE2	2.34	0.51
1:A:553:GLN:HB2	1:A:564:ARG:HB2	1.91	0.51
1:B:301:PRO:HG3	1:B:360:TRP:CE2	2.45	0.51
1:G:553:GLN:HB2	1:G:564:ARG:HB2	1.91	0.51
3:H:221:SER:O	3:H:222:GLN:C	2.48	0.51
3:H:723:VAL:HG11	3:H:742:LYS:HZ3	1.76	0.51
1:A:301:PRO:HG3	1:A:360:TRP:CE2	2.45	0.51
1:G:297:LYS:NZ	1:G:593:GLU:O	2.42	0.51
1:G:321:ALA:HB3	1:G:375:LEU:HD11	1.92	0.51
1:G:374:SER:OG	1:G:385:ILE:O	2.28	0.51
1:J:161:THR:HB	1:J:188:VAL:CG1	2.37	0.51
1:G:548:LYS:NZ	1:G:549:TYR:O	2.42	0.51
1:J:275:SER:OG	1:J:573:TRP:NE1	2.44	0.51
3:F:437:ALA:HB2	3:F:514:PRO:CG	2.41	0.51
3:I:413:ASP:O	3:I:416:MET:HG3	2.10	0.51
3:C:245:ILE:CA	3:C:248:VAL:HG12	2.41	0.51
1:A:22:LYS:HE3	1:B:8:GLN:HE22	1.76	0.51
1:A:237:LEU:HD13	1:A:241:ASP:HB2	1.93	0.51
1:B:275:SER:OG	1:B:573:TRP:NE1	2.44	0.51
1:B:321:ALA:HB3	1:B:375:LEU:HD11	1.92	0.51
3:F:258:GLU:HB2	3:F:259:PRO:HD3	1.93	0.51
3:I:437:ALA:HA	3:I:513:TRP:CZ3	2.38	0.51
3:C:665:PHE:HD1	3:C:665:PHE:C	1.98	0.51
3:C:699:ARG:O	3:C:703:ILE:HG12	2.10	0.51
3:C:706:ALA:HA	3:C:709:ARG:HH21	1.76	0.51
2:E:23:GLU:CB	2:E:25:LYS:HZ1	2.19	0.51
1:B:275:SER:OG	1:B:574:ASP:O	2.25	0.51
1:G:54:SER:CB	3:I:128:ARG:HH22	2.24	0.51
3:F:419:PHE:CD2	3:F:461:GLU:HG2	2.45	0.51
3:H:298:CYS:HA	3:H:301:LYS:HG2	1.93	0.51
3:H:388:LEU:HD22	3:H:422:MET:SD	2.51	0.51
3:H:596:THR:O	3:H:596:THR:HG22	2.11	0.51
3:C:298:CYS:HA	3:C:301:LYS:HG2	1.93	0.51
3:I:258:GLU:HB2	3:I:259:PRO:HD3	1.93	0.50
1:A:237:LEU:HB2	1:A:238:PRO:HD2	1.94	0.50
3:H:455:ILE:CG2	3:H:470:LEU:HD21	2.24	0.50
3:I:298:CYS:HA	3:I:301:LYS:HG2	1.93	0.50



	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
3:C:723:VAL:HG11	3:C:742:LYS:HZ3	1.77	0.50
1:B:65:SER:N	1:B:68:LYS:HZ1	2.07	0.50
3:H:522:CYS:HB2	3:H:622:ILE:HB	1.93	0.50
3:H:559:LEU:O	3:H:592:LEU:N	2.39	0.50
3:I:723:VAL:HG11	3:I:742:LYS:HZ3	1.77	0.50
3:C:606:ASN:HD21	2:E:22:PHE:HD2	1.57	0.50
3:C:596:THR:HG22	3:C:596:THR:O	2.12	0.50
1:A:275:SER:OG	1:A:573:TRP:NE1	2.44	0.50
1:J:321:ALA:HB3	1:J:375:LEU:HD11	1.92	0.50
3:F:238:GLU:O	3:F:242:ASN:ND2	2.32	0.50
3:F:596:THR:O	3:F:596:THR:HG22	2.12	0.50
3:I:626:GLU:HA	3:I:629:ARG:CD	2.18	0.50
2:E:20:LYS:HE3	2:E:23:GLU:HG2	1.93	0.50
3:F:496:VAL:HA	3:F:501:VAL:HA	1.94	0.50
3:I:446:VAL:HG23	3:I:447:SER:H	1.76	0.50
1:J:190:LYS:CG	1:J:193:THR:HG22	2.38	0.50
3:F:225:LEU:HB2	3:F:272:HIS:HE1	1.73	0.50
3:F:225:LEU:HD12	3:F:276:ILE:HD13	1.93	0.50
1:A:374:SER:OG	1:A:385:ILE:O	2.28	0.50
2:D:31:ALA:N	3:F:506:ARG:O	2.34	0.50
2:D:77:HIS:CD2	2:D:96:LEU:HD13	2.47	0.50
1:A:522:ASP:OD1	1:A:522:ASP:N	2.43	0.50
1:B:181:LEU:HD22	1:B:219:GLN:HB3	1.92	0.50
1:J:33:ILE:HD11	1:J:72:VAL:HG22	1.93	0.50
1:J:297:LYS:NZ	1:J:593:GLU:O	2.43	0.50
3:H:218:GLN:O	3:H:221:SER:HB3	2.12	0.50
3:H:706:ALA:HA	3:H:709:ARG:HH21	1.77	0.50
3:I:596:THR:HG22	3:I:596:THR:O	2.12	0.49
3:I:470:LEU:CD1	3:I:474:PHE:CE2	2.81	0.49
3:C:258:GLU:HB2	3:C:259:PRO:HD3	1.93	0.49
3:C:325:GLY:HA3	3:C:377:PHE:CD1	2.47	0.49
1:A:210:SER:HA	1:A:213:LEU:HB2	1.94	0.49
1:J:522:ASP:OD1	1:J:522:ASP:N	2.43	0.49
3:F:298:CYS:HA	3:F:301:LYS:HG2	1.93	0.49
3:H:255:SER:O	3:H:257:GLU:N	2.46	0.49
2:L:20:LYS:HE3	2:L:23:GLU:HG2	1.93	0.49
1:A:8:GLN:NE2	1:B:18:LEU:HB3	2.28	0.49
3:I:717:MET:HB3	3:I:722:LEU:H	1.77	0.49
1:G:431:ILE:HB	1:G:442:TYR:HB3	1.95	0.49
3:I:697:ASP:HA	3:I:700:LYS:HD2	1.94	0.49
3:F:477:MET:HE3	3:F:513:TRP:CZ2	2.47	0.49



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:K:20:LYS:HE3	2:K:23:GLU:HG2	1.94	0.49
1:G:422:SER:OG	1:G:434:MET:O	2.24	0.49
3:F:255:SER:O	3:F:257:GLU:N	2.46	0.49
2:L:84:ILE:HG12	2:L:101:TRP:CE2	2.48	0.49
1:J:374:SER:OG	1:J:385:ILE:O	2.28	0.49
3:H:128:ARG:O	3:H:132:GLN:HB2	2.13	0.49
3:H:258:GLU:HB2	3:H:259:PRO:HD3	1.93	0.49
3:H:559:LEU:HD11	2:K:22:PHE:HB3	1.95	0.49
3:I:506:ARG:O	2:L:31:ALA:N	2.35	0.49
3:C:451:GLU:O	3:C:455:ILE:HG22	2.13	0.49
2:E:35:TRP:CD1	2:E:75:CYS:O	2.65	0.49
1:A:399:VAL:HG12	1:A:414:PRO:HA	1.95	0.49
1:J:37:VAL:HG21	1:J:82:LEU:HD23	1.95	0.49
2:D:20:LYS:HE3	2:D:23:GLU:HG2	1.93	0.49
3:H:491:LEU:C	3:H:493:ALA:H	2.15	0.49
3:C:560:ASN:CB	2:E:25:LYS:HG2	2.31	0.49
1:A:212:TYR:C	1:A:214:SER:H	2.16	0.49
1:B:160:PHE:HE2	1:B:169:PHE:CE2	2.31	0.49
1:J:431:ILE:HB	1:J:442:TYR:HB3	1.95	0.49
2:K:35:TRP:CD1	2:K:75:CYS:O	2.65	0.49
1:A:9:ILE:HG23	1:B:93:ASN:HD21	1.78	0.48
1:J:268:MET:HB3	1:J:287:CYS:SG	2.53	0.48
3:C:559:LEU:HD11	2:E:22:PHE:HB3	1.95	0.48
1:A:161:THR:HB	1:A:188:VAL:CG1	2.37	0.48
3:C:446:VAL:HG23	3:C:447:SER:H	1.76	0.48
1:A:431:ILE:HB	1:A:442:TYR:HB3	1.95	0.48
1:B:455:ARG:NH1	1:B:500:GLU:OE2	2.46	0.48
1:G:455:ARG:NH1	1:G:500:GLU:OE2	2.46	0.48
1:J:48:VAL:HG21	1:J:90:TYR:CZ	2.49	0.48
3:F:77:LEU:HD22	3:F:123:LEU:HD22	1.95	0.48
3:F:626:GLU:HA	3:F:629:ARG:CD	2.18	0.48
3:H:598:GLN:HB3	3:H:634:LEU:HD11	1.95	0.48
2:K:47:ASN:ND2	2:K:54:ILE:HG23	2.24	0.48
3:I:700:LYS:O	3:I:703:ILE:HG12	2.13	0.48
3:I:711:MET:HA	3:I:714:ARG:HB2	1.95	0.48
3:C:255:SER:O	3:C:257:GLU:N	2.46	0.48
1:G:399:VAL:HG13	1:G:415:LEU:HD21	1.94	0.48
1:G:455:ARG:NH1	1:G:457:THR:O	2.47	0.48
3:F:245:ILE:CA	3:F:248:VAL:HG12	2.41	0.48
3:I:128:ARG:O	3:I:132:GLN:HB2	2.13	0.48
3:I:629:ARG:O	3:I:632:GLN:HG3	2.14	0.48


	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:I:706:ALA:HA	3:I:709:ARG:HH21	1.77	0.48
2:L:27:TRP:CE2	2:L:29:ALA:HB2	2.49	0.48
3:C:128:ARG:O	3:C:132:GLN:HB2	2.13	0.48
1:A:144:SER:CB	3:C:133:GLN:HG2	2.44	0.48
2:D:27:TRP:CE2	2:D:29:ALA:HB2	2.49	0.48
3:H:77:LEU:HD22	3:H:123:LEU:HD22	1.95	0.48
1:G:18:LEU:HB3	1:J:8:GLN:NE2	2.28	0.48
1:G:529:VAL:O	1:G:530:ILE:HG13	2.14	0.48
1:J:455:ARG:NH1	1:J:457:THR:O	2.47	0.48
2:D:35:TRP:CD1	2:D:75:CYS:O	2.65	0.48
3:F:598:GLN:HB3	3:F:634:LEU:HD11	1.95	0.48
3:F:703:ILE:HB	3:F:741:ILE:HD13	1.95	0.48
3:H:214:ALA:HA	3:H:267:GLU:CD	2.34	0.48
3:I:614:GLU:HA	3:I:617:GLN:HG2	1.96	0.48
2:L:35:TRP:CD1	2:L:75:CYS:O	2.65	0.48
1:J:397:ARG:CD	1:J:417:CYS:HA	2.40	0.48
1:J:455:ARG:NH1	1:J:500:GLU:OE2	2.46	0.48
2:D:89:LYS:HB3	3:F:768:ALA:HB1	1.96	0.48
3:F:198:ARG:O	3:F:202:GLU:HB3	2.14	0.48
3:F:629:ARG:O	3:F:632:GLN:HG3	2.14	0.48
2:K:27:TRP:CE2	2:K:29:ALA:HB2	2.49	0.48
1:A:455:ARG:NH1	1:A:457:THR:O	2.47	0.48
1:J:413:SER:HB3	1:J:442:TYR:HE1	1.79	0.48
2:D:23:GLU:CB	2:D:25:LYS:HZ1	2.25	0.48
3:H:187:CYS:HB2	3:H:201:TYR:OH	2.14	0.48
3:H:614:GLU:HA	3:H:617:GLN:HG2	1.96	0.48
3:I:337:ASN:O	3:I:338:PRO:C	2.52	0.48
3:I:433:LYS:HB3	3:I:433:LYS:HE3	1.45	0.48
3:I:559:LEU:HD11	2:L:22:PHE:HB3	1.95	0.48
1:B:455:ARG:NH1	1:B:457:THR:O	2.47	0.48
1:G:318:ILE:HB	1:G:353:PHE:HB3	1.95	0.48
3:C:644:LEU:HD11	3:C:659:PHE:HB3	1.96	0.48
3:C:698:ASP:HA	3:C:701:HIS:CD2	2.48	0.48
1:A:368:PHE:HB3	1:A:389:SER:O	2.14	0.48
1:G:48:VAL:HG21	1:G:90:TYR:CZ	2.49	0.48
1:G:413:SER:HB3	1:G:442:TYR:HE1	1.79	0.48
1:G:434:MET:HE2	1:G:455:ARG:HG3	1.96	0.48
3:C:712:LYS:NZ	3:C:767:VAL:O	2.40	0.48
1:J:425:VAL:HB	1:J:466:ALA:HB2	1.96	0.47
1:J:529:VAL:O	1:J:530:ILE:HG13	2.14	0.47
3:F:393:ASP:HB2	3:F:435:HIS:CD2	2.49	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:559:LEU:O	3:F:592:LEU:N	2.39	0.47
3:F:644:LEU:HD11	3:F:659:PHE:HB3	1.96	0.47
3:H:458:LEU:HB3	3:H:467:THR:CG2	2.42	0.47
3:H:605:PHE:HE1	3:H:611:TYR:HB2	1.79	0.47
3:H:629:ARG:O	3:H:632:GLN:HG3	2.14	0.47
3:C:682:GLY:O	3:C:683:GLU:HG2	2.14	0.47
2:E:27:TRP:CE2	2:E:29:ALA:HB2	2.49	0.47
1:B:305:LEU:HB2	1:B:325:VAL:HB	1.96	0.47
1:G:37:VAL:HG13	1:G:77:VAL:HG23	1.96	0.47
1:G:47:MET:O	1:G:51:THR:HG23	2.15	0.47
3:F:614:GLU:HA	3:F:617:GLN:HG2	1.96	0.47
3:F:682:GLY:O	3:F:683:GLU:HG2	2.14	0.47
3:H:644:LEU:HD11	3:H:659:PHE:HB3	1.96	0.47
3:I:470:LEU:HD11	3:I:474:PHE:CD2	2.47	0.47
3:I:559:LEU:O	3:I:592:LEU:N	2.39	0.47
3:C:614:GLU:HA	3:C:617:GLN:HG2	1.96	0.47
3:C:629:ARG:O	3:C:632:GLN:HG3	2.14	0.47
3:F:420:ARG:HA	3:F:461:GLU:OE2	2.14	0.47
3:F:605:PHE:HE1	3:F:611:TYR:HB2	1.79	0.47
3:H:338:PRO:HB3	3:H:387:TYR:CG	2.48	0.47
3:I:689:LYS:HD2	3:I:689:LYS:HA	1.49	0.47
3:C:684:SER:O	3:C:688:ARG:HB2	2.14	0.47
1:G:305:LEU:HB2	1:G:325:VAL:HB	1.97	0.47
1:G:393:GLU:HB2	1:G:396:ARG:HA	1.95	0.47
1:J:305:LEU:HB2	1:J:325:VAL:HB	1.96	0.47
3:F:723:VAL:HG11	3:F:742:LYS:HZ3	1.79	0.47
3:H:346:LEU:CB	3:H:418:LEU:CD1	2.92	0.47
3:H:470:LEU:CD1	3:H:474:PHE:CE2	2.81	0.47
3:I:169:ILE:HG12	3:I:209:PHE:HE1	1.79	0.47
3:C:605:PHE:HE1	3:C:611:TYR:HB2	1.79	0.47
1:A:425:VAL:HB	1:A:466:ALA:HB2	1.96	0.47
1:A:529:VAL:O	1:A:530:ILE:HG13	2.14	0.47
1:G:51:THR:HG21	1:J:17:LEU:HD12	1.96	0.47
1:G:304:ASP:OD1	1:G:304:ASP:N	2.47	0.47
3:H:682:GLY:O	3:H:683:GLU:HG2	2.14	0.47
1:A:305:LEU:HB2	1:A:325:VAL:HB	1.96	0.47
1:A:455:ARG:NH1	1:A:500:GLU:OE2	2.46	0.47
1:G:350:PHE:HD2	1:G:363:LYS:HB2	1.80	0.47
3:F:214:ALA:HA	3:F:267:GLU:CD	2.34	0.47
3:H:712:LYS:NZ	3:H:767:VAL:O	2.40	0.47
3:I:47:LYS:HA	3:I:47:LYS:HD2	1.44	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:I:458:LEU:HB3	3:I:467:THR:CG2	2.41	0.47
3:C:345:LEU:HG	3:C:418:LEU:HD22	1.96	0.47
3:C:598:GLN:HB3	3:C:634:LEU:HD11	1.95	0.47
1:A:265:LYS:HD3	1:A:587:TYR:OH	2.15	0.47
1:A:318:ILE:HB	1:A:353:PHE:HB3	1.95	0.47
1:B:134:VAL:HG21	1:B:169:PHE:HA	1.96	0.47
1:B:160:PHE:CE2	1:B:169:PHE:CE2	3.02	0.47
1:B:304:ASP:OD1	1:B:304:ASP:N	2.47	0.47
1:B:530:ILE:HB	1:B:564:ARG:HH12	1.78	0.47
1:J:265:LYS:HD3	1:J:587:TYR:OH	2.15	0.47
1:J:318:ILE:HB	1:J:353:PHE:HB3	1.95	0.47
3:F:363:ASP:HB3	3:F:366:PHE:HD1	1.79	0.47
3:F:446:VAL:HG23	3:F:447:SER:H	1.76	0.47
3:F:609:GLU:HG3	3:F:610:LYS:H	1.80	0.47
3:I:77:LEU:HD22	3:I:123:LEU:HD22	1.95	0.47
3:I:339:VAL:HA	3:I:391:PHE:HD1	1.80	0.47
3:I:598:GLN:HB3	3:I:634:LEU:HD11	1.95	0.47
3:C:559:LEU:O	3:C:592:LEU:N	2.39	0.47
1:A:304:ASP:OD1	1:A:304:ASP:N	2.47	0.47
1:B:302:PRO:HG2	1:B:305:LEU:HB3	1.97	0.47
1:G:265:LYS:HD3	1:G:587:TYR:OH	2.15	0.47
3:I:682:GLY:O	3:I:683:GLU:HG2	2.14	0.47
1:A:195:ARG:HG3	1:A:224:ALA:HB1	1.97	0.47
1:B:390:VAL:CG1	1:B:393:GLU:HG3	2.43	0.47
1:G:227:GLU:HB3	1:G:228:VAL:H	1.63	0.47
2:D:22:PHE:HB3	3:F:559:LEU:HD11	1.95	0.47
3:F:398:LYS:HA	3:F:398:LYS:HD3	1.53	0.47
3:H:245:ILE:CA	3:H:248:VAL:HG12	2.41	0.47
3:I:609:GLU:HG3	3:I:610:LYS:H	1.80	0.47
3:C:374:PHE:O	3:C:421:PHE:HB3	2.15	0.47
1:A:144:SER:CB	3:C:129:VAL:HG23	2.45	0.47
1:A:326:PRO:HA	1:A:344:PHE:HA	1.97	0.47
1:B:425:VAL:HB	1:B:466:ALA:HB2	1.96	0.47
1:J:326:PRO:HA	1:J:344:PHE:HA	1.98	0.47
1:A:8:GLN:HE22	1:B:18:LEU:HB3	1.80	0.46
1:G:425:VAL:HB	1:G:466:ALA:HB2	1.96	0.46
1:J:202:LEU:HD22	1:J:213:LEU:HG	1.96	0.46
3:C:77:LEU:HD22	3:C:123:LEU:HD22	1.96	0.46
1:A:265:LYS:HE2	1:A:265:LYS:HA	1.98	0.46
1:B:265:LYS:HE2	1:B:265:LYS:HA	1.98	0.46
1:J:275:SER:OG	1:J:574:ASP:O	2.25	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:304:ASP:N	1:J:304:ASP:OD1	2.47	0.46
3:F:346:LEU:CD1	3:F:414:LYS:HB3	2.46	0.46
3:C:623:PRO:HB2	3:C:624:GLU:H	1.63	0.46
1:B:161:THR:HB	1:B:188:VAL:CG1	2.37	0.46
1:B:171:GLN:HA	1:B:171:GLN:OE1	2.15	0.46
1:B:265:LYS:HD3	1:B:587:TYR:OH	2.15	0.46
3:H:336:LYS:HE3	3:H:387:TYR:CE2	2.50	0.46
3:C:525:PRO:HB2	3:C:528:PRO:HD2	1.96	0.46
3:C:692:ARG:HA	3:C:692:ARG:HD3	1.66	0.46
1:J:353:PHE:HB2	1:J:360:TRP:CH2	2.51	0.46
3:I:644:LEU:HD11	3:I:659:PHE:HB3	1.96	0.46
3:C:393:ASP:HA	3:C:439:ARG:NH2	2.25	0.46
3:C:395:LYS:HA	3:C:395:LYS:HD3	1.70	0.46
1:B:318:ILE:HB	1:B:353:PHE:HB3	1.95	0.46
3:H:215:GLU:O	3:H:216:PHE:C	2.54	0.46
3:H:395:LYS:HA	3:H:395:LYS:HD3	1.59	0.46
3:I:605:PHE:HE1	3:I:611:TYR:HB2	1.79	0.46
3:C:646:LYS:HE3	3:C:659:PHE:HE1	1.80	0.46
1:J:434:MET:HE2	1:J:455:ARG:HG3	1.97	0.46
3:F:477:MET:HE3	3:F:513:TRP:CH2	2.51	0.46
3:H:429:GLU:HG2	3:H:466:PHE:HB3	1.98	0.46
3:I:509:THR:HG23	2:L:76:ASN:HD22	1.80	0.46
1:G:326:PRO:HA	1:G:344:PHE:HA	1.97	0.46
3:F:646:LYS:HE3	3:F:659:PHE:HE1	1.80	0.46
1:B:422:SER:OG	1:B:434:MET:O	2.24	0.46
1:B:434:MET:HE2	1:B:455:ARG:HG3	1.98	0.46
1:G:220:ILE:HG13	1:G:220:ILE:O	2.15	0.46
1:J:302:PRO:HG2	1:J:305:LEU:HB3	1.97	0.46
3:I:425:LYS:CE	3:I:462:CYS:SG	3.04	0.46
3:C:516:GLN:HE21	3:C:516:GLN:HB3	1.48	0.46
1:A:51:THR:HG21	1:B:17:LEU:HD13	1.93	0.46
1:A:302:PRO:HG2	1:A:305:LEU:HB3	1.97	0.46
1:B:301:PRO:HB2	1:B:302:PRO:HD3	1.98	0.46
1:B:353:PHE:HB2	1:B:360:TRP:CH2	2.51	0.46
1:G:265:LYS:HA	1:G:265:LYS:HE2	1.98	0.46
1:G:353:PHE:HB2	1:G:360:TRP:CH2	2.51	0.46
3:F:198:ARG:HH21	3:F:202:GLU:HG3	1.80	0.46
3:F:503:LEU:HD21	3:F:531:ALA:CB	2.39	0.46
3:H:703:ILE:HB	3:H:741:ILE:HD13	1.97	0.46
3:I:520:PRO:HG2	3:I:552:HIS:H	1.80	0.46
3:I:646:LYS:HE3	3:I:659:PHE:HE1	1.80	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:455:ILE:HA	3:C:458:LEU:HB2	1.98	0.46
3:C:723:VAL:HA	3:C:726:VAL:HG12	1.98	0.46
1:J:350:PHE:HD2	1:J:363:LYS:HB2	1.80	0.46
3:I:438:ARG:HD2	3:I:438:ARG:HA	1.52	0.46
3:C:207:ALA:HB3	3:C:208:PRO:HD3	1.98	0.46
3:C:215:GLU:OE1	3:C:215:GLU:N	2.49	0.46
3:F:148:ARG:HH11	3:F:200:VAL:HG21	1.81	0.45
3:H:723:VAL:HA	3:H:726:VAL:HG12	1.98	0.45
3:C:346:LEU:HD11	3:C:414:LYS:CB	2.46	0.45
3:C:609:GLU:HG3	3:C:610:LYS:H	1.80	0.45
1:A:265:LYS:CD	1:A:587:TYR:CZ	3.00	0.45
1:A:350:PHE:HD2	1:A:363:LYS:HB2	1.80	0.45
1:B:48:VAL:HG21	1:B:90:TYR:CZ	2.51	0.45
1:B:198:ALA:HB1	1:B:216:VAL:HG12	1.98	0.45
1:B:297:LYS:HZ3	1:B:595:PRO:HD3	1.80	0.45
1:B:350:PHE:HD2	1:B:363:LYS:HB2	1.80	0.45
1:J:402:TYR:HB2	1:J:409:TRP:CZ3	2.51	0.45
1:A:146:GLU:HG2	3:C:133:GLN:OE1	2.16	0.45
1:B:66:GLU:HG2	3:F:54:PHE:HB3	1.98	0.45
1:G:222:ILE:HG12	1:G:257:PHE:CD1	2.51	0.45
1:J:265:LYS:HA	1:J:265:LYS:HE2	1.98	0.45
3:H:609:GLU:HG3	3:H:610:LYS:H	1.80	0.45
1:A:353:PHE:HB2	1:A:360:TRP:CH2	2.51	0.45
1:B:265:LYS:HE2	1:B:585:LYS:HB3	1.99	0.45
3:H:425:LYS:CE	3:H:462:CYS:SG	3.04	0.45
3:I:560:ASN:CB	2:L:25:LYS:HG2	2.30	0.45
3:C:148:ARG:HH11	3:C:200:VAL:HG21	1.80	0.45
3:C:748:LEU:HD13	3:C:748:LEU:HA	1.75	0.45
2:E:88:LEU:HD22	2:E:88:LEU:HA	1.76	0.45
1:B:160:PHE:HE2	1:B:169:PHE:CZ	2.10	0.45
1:G:265:LYS:CD	1:G:587:TYR:CZ	3.00	0.45
1:G:301:PRO:HB2	1:G:302:PRO:HD3	1.99	0.45
3:H:560:ASN:CB	2:K:25:LYS:HG2	2.31	0.45
1:A:237:LEU:HB2	1:A:238:PRO:CD	2.46	0.45
1:A:434:MET:HE2	1:A:455:ARG:HG3	1.97	0.45
1:B:57:ARG:O	1:B:61:MET:HB2	2.17	0.45
1:B:128:ILE:HG12	1:B:136:LEU:HD21	1.99	0.45
1:J:287:CYS:SG	1:J:288:TYR:N	2.90	0.45
3:H:749:ILE:HD13	3:H:758:PRO:HD3	1.98	0.45
2:E:23:GLU:C	2:E:25:LYS:HZ1	2.20	0.45
1:A:37:VAL:HG21	1:A:82:LEU:HD23	1.99	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:156:VAL:O	1:B:160:PHE:HB3	2.17	0.45
1:B:231:ARG:HD2	1:B:231:ARG:N	2.32	0.45
1:J:265:LYS:CD	1:J:587:TYR:CZ	3.00	0.45
1:J:376:VAL:N	1:J:383:TYR:O	2.45	0.45
1:J:566:HIS:O	1:J:566:HIS:ND1	2.50	0.45
3:F:213:SER:O	3:F:214:ALA:C	2.55	0.45
3:F:440:LEU:HB2	3:F:513:TRP:CH2	2.50	0.45
3:F:520:PRO:HG2	3:F:552:HIS:H	1.81	0.45
3:H:473:MET:CG	3:H:512:TYR:HB3	2.47	0.45
3:C:223:LYS:HE3	3:C:227:GLU:HG3	1.99	0.45
1:A:287:CYS:SG	1:A:288:TYR:N	2.90	0.45
1:A:566:HIS:O	1:A:566:HIS:ND1	2.50	0.45
1:B:84:ILE:HA	1:B:87:THR:HG22	1.99	0.45
1:B:326:PRO:HA	1:B:344:PHE:HA	1.98	0.45
1:G:265:LYS:HE2	1:G:585:LYS:HB3	1.99	0.45
1:G:302:PRO:HG2	1:G:305:LEU:HB3	1.97	0.45
1:J:231:ARG:HD2	1:J:231:ARG:N	2.32	0.45
1:J:265:LYS:HE2	1:J:585:LYS:HB3	1.99	0.45
2:D:23:GLU:C	2:D:25:LYS:HZ1	2.20	0.45
3:F:689:LYS:HD2	3:F:689:LYS:HA	1.41	0.45
3:I:703:ILE:HB	3:I:741:ILE:HD13	1.99	0.45
2:L:23:GLU:CB	2:L:25:LYS:HZ1	2.28	0.45
2:L:41:ASN:HD21	2:L:46:ARG:HD2	1.79	0.45
3:C:419:PHE:HE1	3:C:425:LYS:HB2	1.82	0.45
1:G:128:ILE:HG23	1:G:136:LEU:HD21	1.99	0.45
1:J:156:VAL:O	1:J:160:PHE:HB3	2.17	0.45
3:F:425:LYS:HE2	3:F:425:LYS:HB3	1.37	0.45
3:F:714:ARG:NH1	3:F:725:GLU:OE2	2.50	0.45
3:H:213:SER:O	3:H:214:ALA:C	2.55	0.45
3:H:338:PRO:HB3	3:H:387:TYR:HA	1.99	0.45
3:I:723:VAL:HA	3:I:726:VAL:HG12	1.98	0.45
3:C:436:LEU:HD23	3:C:439:ARG:HH11	1.82	0.45
1:A:275:SER:OG	1:A:574:ASP:O	2.26	0.45
1:B:128:ILE:HG23	1:B:136:LEU:HD21	1.99	0.45
1:G:287:CYS:SG	1:G:288:TYR:N	2.90	0.45
1:J:539:ARG:HH22	1:J:577:ARG:HD3	1.82	0.45
3:F:230:ALA:HB2	3:F:276:ILE:HG13	1.99	0.45
3:F:694:LYS:HD2	3:F:694:LYS:HA	1.63	0.45
3:H:697:ASP:HA	3:H:700:LYS:HD2	1.98	0.45
3:I:714:ARG:HB3	3:I:715:LYS:H	1.61	0.45
3:C:455:ILE:HG12	3:C:459:LYS:HG2	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:265:LYS:CD	1:B:587:TYR:CZ	3.00	0.44
1:G:12:GLU:HA	1:G:15:VAL:CG2	2.47	0.44
1:G:255:LYS:HE2	1:G:255:LYS:HB2	1.70	0.44
2:D:25:LYS:HG2	3:F:560:ASN:CB	2.31	0.44
3:F:436:LEU:HD23	3:F:439:ARG:HH11	1.82	0.44
3:C:731:LYS:HD3	3:C:731:LYS:HA	1.49	0.44
1:A:376:VAL:N	1:A:383:TYR:O	2.45	0.44
3:F:440:LEU:CD1	3:F:513:TRP:CH2	3.00	0.44
2:K:23:GLU:C	2:K:25:LYS:HZ1	2.21	0.44
3:I:592:LEU:HD23	3:I:672:VAL:HG13	1.99	0.44
3:C:376:TYR:O	3:C:379:ASN:HB2	2.17	0.44
3:C:714:ARG:NH1	3:C:725:GLU:OE2	2.50	0.44
2:E:98:ASN:HD22	2:E:98:ASN:HA	1.58	0.44
1:B:566:HIS:O	1:B:566:HIS:ND1	2.50	0.44
1:G:62:SER:HA	3:I:118:MET:HG2	2.00	0.44
1:G:78:ASP:OD1	1:G:79:ALA:N	2.51	0.44
1:J:128:ILE:HG23	1:J:136:LEU:HD21	1.99	0.44
3:H:225:LEU:HB2	3:H:272:HIS:CE1	2.52	0.44
3:H:436:LEU:HD23	3:H:439:ARG:HH11	1.82	0.44
2:K:88:LEU:HD22	2:K:92:GLN:HA	1.98	0.44
3:I:396:LEU:HD23	3:I:439:ARG:NH1	2.33	0.44
1:B:287:CYS:SG	1:B:288:TYR:N	2.90	0.44
1:B:539:ARG:HH22	1:B:577:ARG:HD3	1.83	0.44
1:G:397:ARG:O	1:G:414:PRO:HB2	2.18	0.44
1:J:128:ILE:HG12	1:J:136:LEU:HD21	1.99	0.44
1:J:301:PRO:HB2	1:J:302:PRO:HD3	1.99	0.44
3:I:204:ASP:O	3:I:208:PRO:HD2	2.17	0.44
3:I:230:ALA:HB2	3:I:276:ILE:HG13	1.99	0.44
3:I:346:LEU:HD12	3:I:346:LEU:HA	1.73	0.44
3:I:476:ASP:OD1	3:I:508:LEU:HD22	2.17	0.44
3:I:692:ARG:HD3	3:I:692:ARG:HA	1.62	0.44
1:A:301:PRO:HB2	1:A:302:PRO:HD3	1.99	0.44
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.78	0.44
1:G:287:CYS:N	1:G:296:TYR:O	2.41	0.44
1:G:566:HIS:O	1:G:566:HIS:ND1	2.50	0.44
3:F:692:ARG:HD3	3:F:692:ARG:HA	1.50	0.44
3:I:707:ILE:HG12	3:I:726:VAL:HG21	2.00	0.44
3:C:265:GLU:HB3	3:C:306:VAL:HG22	2.00	0.44
3:C:632:GLN:HB2	3:C:636:CYS:HB3	2.00	0.44
1:A:265:LYS:HE2	1:A:585:LYS:HB3	1.99	0.44
1:A:539:ARG:HH22	1:A:577:ARG:HD3	1.82	0.44



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:78:ASP:OD1	1:B:79:ALA:N	2.51	0.44
3:F:592:LEU:HD23	3:F:672:VAL:HG13	1.99	0.44
3:H:230:ALA:HB2	3:H:276:ILE:HG13	1.99	0.44
3:H:476:ASP:OD1	3:H:508:LEU:HD22	2.17	0.44
1:A:128:ILE:HG23	1:A:136:LEU:HD21	1.99	0.44
1:A:388:ASP:C	1:A:390:VAL:N	2.71	0.44
1:J:211:GLN:H	1:J:211:GLN:HG3	1.56	0.44
3:H:113:GLN:O	3:H:117:VAL:HG23	2.18	0.44
3:H:653:ILE:N	3:H:653:ILE:HD13	2.33	0.44
3:H:689:LYS:HD2	3:H:689:LYS:HA	1.65	0.44
3:H:714:ARG:NH1	3:H:725:GLU:OE2	2.50	0.44
3:I:498:LEU:HD13	3:I:498:LEU:HA	1.74	0.44
3:I:634:LEU:HD23	3:I:634:LEU:HA	1.79	0.44
3:C:338:PRO:HA	3:C:341:TYR:CD2	2.52	0.44
3:C:653:ILE:N	3:C:653:ILE:HD13	2.33	0.44
1:A:78:ASP:OD1	1:A:79:ALA:N	2.51	0.44
1:B:211:GLN:H	1:B:211:GLN:HG3	1.37	0.44
1:G:128:ILE:HG12	1:G:136:LEU:HD21	1.99	0.44
1:G:539:ARG:HH22	1:G:577:ARG:HD3	1.83	0.44
1:J:265:LYS:HD2	1:J:587:TYR:CZ	2.53	0.44
3:F:217:PHE:O	3:F:218:GLN:C	2.56	0.44
3:F:265:GLU:HB3	3:F:306:VAL:HG22	2.00	0.44
3:F:390:LEU:HD13	3:F:390:LEU:HA	1.80	0.44
3:F:622:ILE:HG12	3:F:627:LEU:HB2	2.00	0.44
3:H:345:LEU:HG	3:H:418:LEU:HD11	2.00	0.44
3:H:509:THR:HG22	3:H:511:GLY:H	1.83	0.44
3:H:592:LEU:HD23	3:H:672:VAL:HG13	1.99	0.44
3:H:684:SER:O	3:H:688:ARG:HB2	2.17	0.44
2:L:23:GLU:C	2:L:25:LYS:HZ1	2.20	0.44
3:C:230:ALA:HB2	3:C:276:ILE:HG13	1.99	0.44
1:B:37:VAL:HG21	1:B:82:LEU:HD23	1.99	0.44
1:B:265:LYS:HD2	1:B:587:TYR:CZ	2.53	0.44
3:H:632:GLN:HB2	3:H:636:CYS:HB3	2.00	0.44
3:I:731:LYS:HA	3:I:731:LYS:HD3	1.54	0.44
3:C:346:LEU:HD21	3:C:411:ILE:HA	2.00	0.44
2:E:47:ASN:O	2:E:48:HIS:HB2	2.18	0.44
1:A:128:ILE:HG12	1:A:136:LEU:HD21	1.99	0.43
1:A:415:LEU:H	1:A:415:LEU:HG	1.66	0.43
1:B:64:LEU:HB3	1:B:65:SER:H	1.61	0.43
1:G:58:ALA:HB1	3:I:121:ASP:CB	2.45	0.43
3:F:190:LEU:HB3	3:F:201:TYR:HB2	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:H:349:LYS:HE3	3:H:421:PHE:CE2	2.52	0.43
3:H:396:LEU:HD13	3:H:396:LEU:HA	1.81	0.43
3:H:646:LYS:HE3	3:H:659:PHE:HE1	1.80	0.43
3:I:337:ASN:OD1	3:I:339:VAL:HG13	2.17	0.43
3:I:751:ARG:HD2	3:I:751:ARG:HA	1.44	0.43
1:A:156:VAL:O	1:A:160:PHE:HB3	2.17	0.43
1:A:265:LYS:HD2	1:A:587:TYR:CZ	2.53	0.43
1:G:390:VAL:CG1	1:G:393:GLU:HG3	2.43	0.43
1:J:181:LEU:HD21	1:J:220:ILE:HD13	1.99	0.43
3:F:113:GLN:O	3:F:117:VAL:HG23	2.18	0.43
3:F:425:LYS:N	3:F:733:ARG:O	2.50	0.43
3:F:653:ILE:N	3:F:653:ILE:HD13	2.33	0.43
3:F:751:ARG:HA	3:F:751:ARG:HD2	1.47	0.43
3:I:113:GLN:O	3:I:117:VAL:HG23	2.18	0.43
3:I:291:GLY:HA2	3:I:355:PHE:HZ	1.81	0.43
3:I:647:GLU:HB2	3:I:648:PRO:HD3	2.00	0.43
1:A:84:ILE:HA	1:A:87:THR:HG22	1.99	0.43
1:G:265:LYS:HD2	1:G:587:TYR:CZ	2.53	0.43
3:F:723:VAL:HA	3:F:726:VAL:HG12	1.98	0.43
3:F:752:GLU:HB2	3:F:753:TYR:H	1.52	0.43
3:H:707:ILE:HG12	3:H:726:VAL:HG21	2.00	0.43
3:C:86:ILE:HG23	3:C:90:ARG:HD2	2.00	0.43
3:C:153:ARG:HH21	3:C:200:VAL:HG13	1.83	0.43
3:C:225:LEU:HB3	3:C:272:HIS:CE1	2.53	0.43
3:C:592:LEU:HD23	3:C:672:VAL:HG13	1.99	0.43
1:A:22:LYS:NZ	1:B:6:GLU:OE1	2.51	0.43
1:G:13:TYR:CD2	1:G:13:TYR:C	2.92	0.43
3:H:86:ILE:HG23	3:H:90:ARG:HD2	2.00	0.43
3:H:470:LEU:HD11	3:H:474:PHE:CD2	2.47	0.43
3:I:86:ILE:HG23	3:I:90:ARG:HD2	2.00	0.43
3:C:508:LEU:HB3	3:C:513:TRP:CD1	2.54	0.43
3:C:526:PRO:O	3:C:529:ARG:HB2	2.18	0.43
3:C:527:ALA:HB3	3:C:528:PRO:HD3	2.00	0.43
1:A:133:CYS:SG	1:A:134:VAL:N	2.92	0.43
1:A:419:TRP:HZ2	1:A:438:LEU:HD23	1.84	0.43
1:B:160:PHE:HE2	1:B:169:PHE:CD2	2.37	0.43
1:J:133:CYS:SG	1:J:134:VAL:N	2.92	0.43
3:H:221:SER:HA	3:H:272:HIS:NE2	2.33	0.43
3:H:553:HIS:HA	3:H:597:PHE:CE1	2.53	0.43
3:I:414:LYS:HD3	3:I:414:LYS:HA	1.77	0.43
3:I:653:ILE:HD13	3:I:653:ILE:N	2.33	0.43



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:L:47:ASN:O	2:L:48:HIS:HB2	2.18	0.43
3:C:647:GLU:HB2	3:C:648:PRO:HD3	2.00	0.43
1:A:48:VAL:HA	1:A:51:THR:HG22	2.01	0.43
1:A:193:THR:HG23	1:A:194:VAL:N	2.33	0.43
1:A:270:ILE:HD11	1:A:584:GLY:HA3	2.00	0.43
1:J:48:VAL:HA	1:J:51:THR:HG22	2.01	0.43
1:J:233:TRP:HH2	1:J:245:VAL:CG2	2.25	0.43
3:F:647:GLU:HB2	3:F:648:PRO:HD3	2.00	0.43
3:F:707:ILE:HB	3:F:726:VAL:HG21	1.99	0.43
2:K:23:GLU:CB	2:K:25:LYS:HZ1	2.29	0.43
3:C:113:GLN:O	3:C:117:VAL:HG23	2.18	0.43
3:C:248:VAL:O	3:C:256:THR:HG21	2.18	0.43
3:F:269:ILE:HB	3:F:306:VAL:HG21	2.01	0.43
3:F:425:LYS:NZ	3:F:462:CYS:HB2	2.33	0.43
3:H:446:VAL:HG23	3:H:447:SER:H	1.76	0.43
3:H:647:GLU:HB2	3:H:648:PRO:HD3	2.00	0.43
3:I:423:GLN:HG2	3:I:424:GLU:H	1.83	0.43
3:C:414:LYS:HA	3:C:417:VAL:HB	2.00	0.43
3:C:634:LEU:HD23	3:C:634:LEU:HA	1.78	0.43
1:A:268:MET:HB3	1:A:287:CYS:SG	2.58	0.43
1:B:193:THR:HG23	1:B:194:VAL:N	2.34	0.43
1:G:233:TRP:HH2	1:G:245:VAL:CG2	2.25	0.43
3:H:265:GLU:HB3	3:H:306:VAL:HG22	2.00	0.43
3:H:423:GLN:HG2	3:H:424:GLU:H	1.83	0.43
3:I:553:HIS:HA	3:I:597:PHE:CE1	2.53	0.43
3:I:717:MET:HA	3:I:721:VAL:HB	2.00	0.43
1:G:133:CYS:SG	1:G:134:VAL:N	2.91	0.43
3:F:86:ILE:HG23	3:F:90:ARG:HD2	2.00	0.43
3:I:488:ARG:HA	3:I:488:ARG:HD2	1.49	0.43
3:I:715:LYS:HB2	3:I:722:LEU:HD21	2.00	0.43
2:L:52:LEU:HD12	2:L:56:CYS:HB3	2.01	0.43
3:C:346:LEU:CD2	3:C:411:ILE:HA	2.49	0.43
3:C:459:LYS:HZ1	3:C:468:SER:HA	1.84	0.43
3:C:553:HIS:HA	3:C:597:PHE:CE1	2.53	0.43
1:B:133:CYS:SG	1:B:134:VAL:N	2.91	0.42
1:G:268:MET:HB3	1:G:287:CYS:SG	2.59	0.42
1:J:297:LYS:HZ1	1:J:594:SER:HA	1.83	0.42
3:F:553:HIS:HA	3:F:597:PHE:CE1	2.53	0.42
3:H:74:TYR:OH	3:H:137:GLU:OE2	2.37	0.42
3:H:527:ALA:HB3	3:H:528:PRO:HD3	2.00	0.42
2:K:52:LEU:HD12	2:K:56:CYS:HB3	2.01	0.42



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:325:VAL:O	1:A:345:ARG:N	2.50	0.42
3:F:425:LYS:HA	3:F:428:PHE:HB3	2.00	0.42
3:H:269:ILE:HB	3:H:306:VAL:HG21	2.01	0.42
2:K:47:ASN:O	2:K:48:HIS:HB2	2.18	0.42
3:I:265:GLU:HB3	3:I:306:VAL:HG22	2.00	0.42
3:I:345:LEU:HD13	3:I:418:LEU:HD21	2.01	0.42
3:I:491:LEU:HD23	3:I:491:LEU:HA	1.79	0.42
3:I:714:ARG:HA	3:I:714:ARG:HD2	1.75	0.42
3:C:74:TYR:OH	3:C:137:GLU:OE2	2.37	0.42
3:C:691:THR:HA	3:C:694:LYS:HB2	2.01	0.42
1:A:376:VAL:O	1:A:383:TYR:N	2.38	0.42
1:B:286:VAL:HA	1:B:297:LYS:HA	2.01	0.42
3:F:541:ALA:CB	3:H:501:VAL:O	2.61	0.42
3:H:217:PHE:CE2	3:H:264:VAL:HG22	2.54	0.42
3:H:526:PRO:O	3:H:529:ARG:HB2	2.18	0.42
2:K:24:VAL:CA	2:K:25:LYS:HE2	2.41	0.42
3:I:632:GLN:HB2	3:I:636:CYS:HB3	2.00	0.42
1:A:402:TYR:HB2	1:A:409:TRP:CZ3	2.55	0.42
1:B:325:VAL:O	1:B:345:ARG:N	2.50	0.42
1:B:470:LYS:NZ	1:B:503:ASP:OD2	2.47	0.42
1:J:419:TRP:HZ2	1:J:438:LEU:HD23	1.84	0.42
3:F:632:GLN:HB2	3:F:636:CYS:HB3	2.00	0.42
3:H:248:VAL:O	3:H:256:THR:HG21	2.18	0.42
3:H:516:GLN:HE22	3:H:551:GLN:HG3	1.85	0.42
3:C:269:ILE:HB	3:C:306:VAL:HG21	2.01	0.42
3:C:711:MET:HG3	3:C:722:LEU:HD13	1.99	0.42
3:F:285:VAL:CG2	3:F:286:HIS:N	2.83	0.42
1:B:223:ASP:HB3	1:B:257:PHE:HE1	1.85	0.42
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.82	0.42
1:B:402:TYR:HB2	1:B:409:TRP:CZ3	2.54	0.42
1:G:231:ARG:HD2	1:G:231:ARG:N	2.32	0.42
1:J:426:VAL:O	1:J:426:VAL:CG1	2.68	0.42
3:H:484:MET:SD	3:H:504:THR:HA	2.59	0.42
1:A:91:THR:HA	1:B:8:GLN:OE1	2.20	0.42
1:B:160:PHE:CD2	1:B:169:PHE:CD1	3.06	0.42
1:B:554:TYR:HB2	1:B:561:TRP:CD1	2.55	0.42
1:J:397:ARG:HD2	1:J:417:CYS:N	2.33	0.42
3:F:248:VAL:O	3:F:256:THR:HG21	2.18	0.42
3:F:441:LEU:O	3:F:554:MET:SD	2.77	0.42
3:I:74:TYR:OH	3:I:137:GLU:OE2	2.37	0.42
3:I:470:LEU:CD1	3:I:474:PHE:CD2	3.03	0.42



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:385:PRO:HB3	3:C:428:PHE:HB2	2.02	0.42
2:E:52:LEU:HD12	2:E:56:CYS:HB3	2.01	0.42
1:A:225:LEU:HD12	1:A:225:LEU:HA	1.68	0.42
1:A:554:TYR:HB2	1:A:561:TRP:CD1	2.55	0.42
1:G:325:VAL:O	1:G:345:ARG:N	2.50	0.42
1:G:376:VAL:N	1:G:383:TYR:O	2.45	0.42
3:F:451:GLU:HB3	3:F:474:PHE:CE2	2.55	0.42
3:H:287:MET:HE1	3:H:299:MET:SD	2.60	0.42
3:H:408:VAL:O	3:H:411:ILE:HG22	2.19	0.42
3:I:102:LEU:HD12	3:I:102:LEU:C	2.40	0.42
3:I:285:VAL:CG2	3:I:286:HIS:N	2.83	0.42
3:C:733:ARG:HD3	3:C:733:ARG:HA	1.82	0.42
1:A:225:LEU:HG	1:A:230:GLN:HE22	1.84	0.42
1:A:286:VAL:HA	1:A:297:LYS:HA	2.01	0.42
1:A:597:LYS:HA	1:A:598:PRO:HD2	1.91	0.42
1:G:280:CYS:HB3	1:G:281:SER:H	1.71	0.42
1:G:286:VAL:HA	1:G:297:LYS:HA	2.01	0.42
1:G:597:LYS:HA	1:G:598:PRO:HD2	1.91	0.42
1:J:217:LEU:HG	1:J:225:LEU:HD11	2.01	0.42
3:H:383:ARG:HE	3:H:383:ARG:HB2	1.33	0.42
3:I:212:MET:HE3	3:I:212:MET:HB3	1.79	0.42
1:G:221:ARG:HB3	1:G:255:LYS:HE2	2.02	0.42
1:G:539:ARG:HD3	1:G:549:TYR:CZ	2.55	0.42
1:J:325:VAL:O	1:J:345:ARG:N	2.50	0.42
3:F:102:LEU:HD12	3:F:102:LEU:C	2.40	0.42
3:F:593:GLN:HE21	3:F:593:GLN:HB3	1.71	0.42
3:H:102:LEU:HD12	3:H:102:LEU:C	2.40	0.42
3:H:212:MET:HE3	3:H:212:MET:HB3	1.68	0.42
3:H:217:PHE:HB2	3:H:267:GLU:OE1	2.20	0.42
3:H:470:LEU:CD1	3:H:474:PHE:CD2	3.03	0.42
3:I:419:PHE:O	3:I:422:MET:HB2	2.20	0.42
2:E:25:LYS:CE	2:E:25:LYS:CA	2.96	0.42
1:B:102:GLU:HG3	1:B:135:ARG:HH12	1.85	0.41
1:G:41:GLU:H	1:G:41:GLU:HG2	1.42	0.41
1:G:195:ARG:HE	1:G:195:ARG:HB3	1.61	0.41
3:I:526:PRO:HA	3:I:529:ARG:CB	2.49	0.41
3:I:638:LYS:HZ3	3:I:674:ILE:HG23	1.85	0.41
2:L:23:GLU:CB	2:L:25:LYS:NZ	2.83	0.41
3:C:102:LEU:HD12	3:C:102:LEU:C	2.40	0.41
3:C:430:ARG:HE	3:C:434:GLN:HE21	1.67	0.41
3:C:452:LYS:O	3:C:455:ILE:HG23	2.19	0.41



	ious page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:539:ARG:HD3	1:A:549:TYR:CZ	2.55	0.41
1:B:48:VAL:HA	1:B:51:THR:HG22	2.01	0.41
1:G:102:GLU:HG3	1:G:135:ARG:HH12	1.85	0.41
1:G:419:TRP:HZ2	1:G:438:LEU:HD23	1.84	0.41
1:J:87:THR:O	1:J:91:THR:HG22	2.20	0.41
3:F:400:VAL:CG1	3:F:401:LYS:N	2.83	0.41
3:H:285:VAL:HG23	3:H:286:HIS:N	2.35	0.41
3:H:285:VAL:CG2	3:H:286:HIS:N	2.83	0.41
3:I:455:ILE:CG2	3:I:470:LEU:HD21	2.24	0.41
3:I:500:GLY:HA2	3:I:503:LEU:HD23	2.01	0.41
3:C:406:GLN:H	3:C:406:GLN:HG3	1.38	0.41
1:G:554:TYR:HB2	1:G:561:TRP:CD1	2.55	0.41
1:J:539:ARG:HD3	1:J:549:TYR:CZ	2.55	0.41
3:F:285:VAL:HG23	3:F:286:HIS:N	2.35	0.41
3:F:508:LEU:HB3	3:F:513:TRP:CD1	2.55	0.41
3:I:269:ILE:HB	3:I:306:VAL:HG21	2.01	0.41
2:L:41:ASN:ND2	2:L:46:ARG:HD2	2.36	0.41
2:L:52:LEU:HD21	2:L:59:ASN:HA	2.03	0.41
3:C:700:LYS:HG2	3:C:744:ARG:HD2	2.02	0.41
1:A:22:LYS:HZ3	1:B:6:GLU:CD	2.22	0.41
1:G:45:HIS:CG	1:J:47:MET:HE1	2.55	0.41
2:D:84:ILE:HD12	2:D:84:ILE:HA	1.93	0.41
3:F:266:ARG:O	3:F:270:SER:HB2	2.21	0.41
3:F:709:ARG:HE	3:F:709:ARG:HB3	1.34	0.41
3:H:223:LYS:HB3	3:H:223:LYS:HE2	1.25	0.41
3:H:266:ARG:O	3:H:270:SER:HB2	2.21	0.41
3:I:285:VAL:HG23	3:I:286:HIS:N	2.35	0.41
3:I:287:MET:HE1	3:I:299:MET:SD	2.60	0.41
1:A:212:TYR:C	1:A:214:SER:N	2.74	0.41
1:J:286:VAL:HA	1:J:297:LYS:HA	2.01	0.41
1:J:554:TYR:HB2	1:J:561:TRP:CD1	2.55	0.41
3:H:224:PHE:O	3:H:225:LEU:C	2.59	0.41
3:H:374:PHE:O	3:H:378:LEU:HB2	2.20	0.41
3:H:625:ARG:H	3:H:625:ARG:HG2	1.50	0.41
3:I:221:SER:HB2	3:I:272:HIS:NE2	2.35	0.41
3:C:266:ARG:O	3:C:270:SER:HB2	2.21	0.41
3:C:285:VAL:CG2	3:C:286:HIS:N	2.83	0.41
3:C:287:MET:HE1	3:C:299:MET:SD	2.60	0.41
3:C:390:LEU:HD13	3:C:390:LEU:HA	1.75	0.41
2:E:52:LEU:HD21	2:E:59:ASN:HA	2.03	0.41
1:A:87:THR:O	1:A:91:THR:HG22	2.20	0.41



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:419:TRP:HZ2	1:B:438:LEU:HD23	1.84	0.41
3:F:74:TYR:CZ	3:F:142:LEU:HD22	2.56	0.41
3:I:393:ASP:O	3:I:394:ASP:C	2.59	0.41
2:L:41:ASN:ND2	2:L:46:ARG:CG	2.84	0.41
3:C:509:THR:C	2:E:32:LEU:HD11	2.41	0.41
1:A:426:VAL:O	1:A:426:VAL:CG1	2.68	0.41
1:B:212:TYR:O	1:B:216:VAL:HG23	2.20	0.41
1:G:426:VAL:O	1:G:426:VAL:CG1	2.68	0.41
2:D:23:GLU:CB	2:D:25:LYS:NZ	2.83	0.41
3:F:349:LYS:HE2	3:F:421:PHE:CE2	2.53	0.41
3:F:558:ASP:OD1	3:F:671:ARG:NH2	2.54	0.41
3:H:74:TYR:CZ	3:H:142:LEU:HD22	2.56	0.41
3:H:218:GLN:O	3:H:222:GLN:HG2	2.21	0.41
3:I:266:ARG:O	3:I:270:SER:HB2	2.21	0.41
3:C:558:ASP:OD1	3:C:671:ARG:NH2	2.54	0.41
3:H:480:SER:HB3	3:H:508:LEU:HD23	2.03	0.41
3:I:749:ILE:HD13	3:I:758:PRO:HD3	2.02	0.41
3:C:346:LEU:HD11	3:C:414:LYS:HB3	2.03	0.41
3:C:707:ILE:HG13	3:C:711:MET:HG2	2.02	0.41
1:A:102:GLU:HG3	1:A:135:ARG:HH12	1.85	0.41
1:A:457:THR:HG22	1:A:459:ARG:HG2	2.02	0.41
1:B:87:THR:O	1:B:91:THR:HG22	2.21	0.41
1:B:426:VAL:O	1:B:426:VAL:CG1	2.68	0.41
1:G:277:GLU:H	1:G:277:GLU:HG3	1.55	0.41
1:G:457:THR:HG22	1:G:459:ARG:HG2	2.02	0.41
1:J:297:LYS:HZ2	1:J:592:GLU:HG2	1.86	0.41
2:D:31:ALA:O	3:F:507:VAL:HA	2.21	0.41
3:F:346:LEU:HD12	3:F:346:LEU:HA	1.72	0.41
3:H:539:TYR:HE2	3:H:546:ARG:HB2	1.85	0.41
3:H:558:ASP:OD1	3:H:671:ARG:NH2	2.54	0.41
2:K:41:ASN:ND2	2:K:46:ARG:CG	2.84	0.41
3:I:480:SER:HB3	3:I:508:LEU:HD23	2.03	0.41
3:C:524:ILE:HG22	3:C:529:ARG:HG3	2.02	0.41
2:E:41:ASN:ND2	2:E:46:ARG:CG	2.84	0.41
2:E:41:ASN:ND2	2:E:46:ARG:HD2	2.36	0.41
3:F:752:GLU:H	3:F:752:GLU:HG2	1.60	0.41
3:H:682:GLY:C	3:H:683:GLU:OE1	2.60	0.41
2:K:52:LEU:HD21	2:K:59:ASN:HA	2.02	0.41
3:C:285:VAL:HG23	3:C:286:HIS:N	2.35	0.41
3:C:455:ILE:O	3:C:457:LYS:N	2.54	0.41
3:C:619:GLU:H	3:C:619:GLU:HG3	1.64	0.41



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:638:LYS:HG3	3:C:642:ARG:HG2	2.03	0.41
1:A:91:THR:HG23	1:A:93:ASN:HB3	2.03	0.40
1:A:226:SER:HB2	1:A:228:VAL:HG23	2.03	0.40
1:B:81:THR:O	1:B:84:ILE:HG22	2.21	0.40
1:B:238:PRO:HA	1:B:239:PRO:HD3	1.98	0.40
1:B:397:ARG:O	1:B:414:PRO:HB2	2.21	0.40
1:G:45:HIS:CD2	1:J:47:MET:CE	3.04	0.40
1:G:82:LEU:HD12	1:G:82:LEU:HA	1.84	0.40
1:G:402:TYR:HB2	1:G:409:TRP:CZ3	2.57	0.40
1:J:102:GLU:HG3	1:J:135:ARG:HH12	1.85	0.40
1:J:221:ARG:HG2	1:J:255:LYS:HG3	2.03	0.40
3:F:168:MET:SD	3:F:183:ILE:HD11	2.62	0.40
3:H:491:LEU:C	3:H:493:ALA:N	2.75	0.40
3:H:709:ARG:HE	3:H:709:ARG:HB3	1.37	0.40
3:H:752:GLU:HB3	3:H:753:TYR:H	1.72	0.40
3:I:558:ASP:OD1	3:I:671:ARG:NH2	2.54	0.40
3:I:682:GLY:C	3:I:683:GLU:OE1	2.60	0.40
2:L:45:CYS:HB2	2:L:54:ILE:HG12	2.04	0.40
1:B:282:LEU:HB3	1:B:283:TYR:CD2	2.56	0.40
1:B:457:THR:HG22	1:B:459:ARG:HG2	2.02	0.40
1:G:191:GLU:OE1	1:G:223:ASP:HB3	2.22	0.40
1:G:283:TYR:HB2	1:G:306:HIS:ND1	2.36	0.40
1:J:376:VAL:O	1:J:383:TYR:N	2.39	0.40
1:J:457:THR:HG22	1:J:459:ARG:HG2	2.02	0.40
3:F:619:GLU:H	3:F:619:GLU:HG3	1.68	0.40
3:H:512:TYR:CD2	2:K:104:GLN:NE2	2.88	0.40
3:H:703:ILE:HD11	3:H:744:ARG:HD3	2.03	0.40
2:K:23:GLU:CB	2:K:25:LYS:NZ	2.83	0.40
3:I:148:ARG:HH11	3:I:200:VAL:HG21	1.86	0.40
3:I:375:GLU:HA	3:I:421:PHE:O	2.21	0.40
3:I:638:LYS:HG2	3:I:642:ARG:HA	2.03	0.40
3:C:74:TYR:CZ	3:C:142:LEU:HD22	2.56	0.40
1:A:211:GLN:H	1:A:211:GLN:HG3	1.40	0.40
1:B:265:LYS:HD3	1:B:587:TYR:CZ	2.57	0.40
1:B:275:SER:O	1:B:276:SER:C	2.59	0.40
3:F:124:MET:O	3:F:128:ARG:HG2	2.22	0.40
3:F:287:MET:HE1	3:F:299:MET:SD	2.60	0.40
3:F:560:ASN:HA	3:F:591:ILE:HG13	2.03	0.40
3:F:634:LEU:HD23	3:F:634:LEU:HA	1.78	0.40
3:H:200:VAL:O	3:H:201:TYR:C	2.58	0.40
3:H:411:ILE:HD12	3:H:411:ILE:HA	1.86	0.40



	1	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:H:634:LEU:HA	3:H:634:LEU:HD23	1.78	0.40	
3:I:74:TYR:CZ	3:I:142:LEU:HD22	2.56	0.40	
3:I:249:MET:H	3:I:249:MET:HG3	1.77	0.40	
3:I:717:MET:HG2	3:I:722:LEU:HD12	2.02	0.40	
3:C:124:MET:O	3:C:128:ARG:HG2	2.21	0.40	
3:C:168:MET:SD	3:C:183:ILE:HD11	2.62	0.40	
3:C:682:GLY:C	3:C:683:GLU:OE1	2.60	0.40	
1:A:13:TYR:CE2	1:B:92:GLY:HA2	2.57	0.40	
1:A:297:LYS:HZ1	1:A:594:SER:HA	1.85	0.40	
1:B:539:ARG:HD3	1:B:549:TYR:CZ	2.55	0.40	
1:G:198:ALA:HB1	1:G:216:VAL:HG11	2.03	0.40	
1:J:190:LYS:HD3	1:J:192:GLU:HB2	2.02	0.40	
3:F:311:LYS:HE3	3:F:311:LYS:HB3	1.90	0.40	
3:F:638:LYS:HG2	3:F:642:ARG:HA	2.03	0.40	
3:F:682:GLY:C	3:F:683:GLU:OE1	2.60	0.40	
3:H:638:LYS:HG2	3:H:642:ARG:HA	2.03	0.40	
1:A:166:GLN:HB2	1:A:169:PHE:HB3	2.04	0.40	
1:A:244:VAL:O	1:A:247:GLN:HG3	2.21	0.40	
1:G:225:LEU:HD12	1:G:230:GLN:HE22	1.83	0.40	
3:F:414:LYS:HA	3:F:414:LYS:HD3	1.43	0.40	
3:H:168:MET:SD	3:H:183:ILE:HD11	2.62	0.40	
3:H:606:ASN:HD21	2:K:22:PHE:HB2	1.87	0.40	
3:I:393:ASP:HA	3:I:439:ARG:HH21	1.87	0.40	
3:I:700:LYS:HG2	3:I:744:ARG:HD2	2.04	0.40	
3:C:560:ASN:HA	3:C:591:ILE:HG13	2.03	0.40	
3:C:768:ALA:HB1	2:E:89:LYS:HB3	2.03	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	P	erce	entiles
1	А	556/623~(89%)	509 (92%)	44 (8%)	3 (0%)		29	69
1	В	549/623~(88%)	506 (92%)	39 (7%)	4 (1%)		22	63
1	G	556/623~(89%)	495 (89%)	53 (10%)	8 (1%)		11	46
1	J	547/623~(88%)	495 (90%)	49 (9%)	3 (0%)		29	69
2	D	87/121 (72%)	61 (70%)	21 (24%)	5 (6%)		1	18
2	Е	87/121 (72%)	59 (68%)	23 (26%)	5 (6%)		1	18
2	K	87/121 (72%)	60 (69%)	22 (25%)	5 (6%)		1	18
2	L	87/121 (72%)	62 (71%)	20 (23%)	5 (6%)		1	18
3	С	716/776~(92%)	629 (88%)	82 (12%)	5 (1%)		22	63
3	F	716/776~(92%)	610 (85%)	93 (13%)	13 (2%)		8	40
3	Н	716/776~(92%)	615 (86%)	94 (13%)	7 (1%)		15	55
3	Ι	716/776~(92%)	620 (87%)	87 (12%)	9 (1%)		12	48
All	All	5420/6080 (89%)	4721 (87%)	627 (12%)	72 (1%)		16	48

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	390	VAL
1	В	279	PRO
1	G	221	ARG
2	D	68	CYS
3	F	400	VAL
3	F	464	CYS
3	F	465	GLN
3	F	526	PRO
3	F	623	PRO
3	Н	200	VAL
2	Κ	68	CYS
3	Ι	200	VAL
3	Ι	623	PRO
2	L	68	CYS
2	Е	68	CYS
1	G	227	GLU
1	G	254	PRO
3	F	203	GLU
3	F	204	ASP
3	F	399	GLY
3	F	510	THR
3	Ι	510	THR



Mol	Chain	Res	Type
3	Ι	517	SER
3	С	330	SER
3	С	623	PRO
1	А	395	ASN
1	В	144	SER
1	J	252	SER
2	D	44	ILE
2	D	57	GLN
3	F	202	GLU
3	Н	202	GLU
3	Н	215	GLU
3	Ι	442	THR
3	Ι	624	GLU
2	L	57	GLN
3	С	510	THR
3	C	517	SER
1	В	252	SER
1	G	252	SER
1	G	256	PHE
1	G	276	SER
1	J	144	SER
1	J	207	GLU
2	D	35	TRP
2	D	38	VAL
3	F	624	GLU
3	Н	400	VAL
3	Н	753	TYR
2	Κ	35	TRP
2	K	38	VAL
2	K	57	GLN
3	Ι	204	ASP
2	L	35	TRP
2	L	38	VAL
2	E	35	TRP
2	E	38	VAL
2	E	57	GLN
1	В	207	GLU
3	F	206	GLU
3	F	525	PRO
3	Н	517	SER
2	K	48	HIS
3	Ι	199	SER



Continued from previous page...

Mol	Chain	Res	Type
3	Ι	752	GLU
2	L	48	HIS
3	С	380	LEU
2	Е	48	HIS
1	А	252	SER
1	G	220	ILE
3	Н	686	PRO
1	G	253	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	478/560~(85%)	446 (93%)	32~(7%)	16	41
1	В	485/560~(87%)	452 (93%)	33~(7%)	16	41
1	G	470/560~(84%)	427 (91%)	43~(9%)	9	29
1	J	491/560~(88%)	452 (92%)	39~(8%)	12	35
2	D	66/102~(65%)	58~(88%)	8 (12%)	5	20
2	Ε	78/102~(76%)	66~(85%)	12 (15%)	2	14
2	Κ	78/102~(76%)	66~(85%)	12 (15%)	2	14
2	L	78/102~(76%)	67~(86%)	11 (14%)	3	16
3	С	621/701~(89%)	542 (87%)	79~(13%)	4	18
3	F	597/701~(85%)	520 (87%)	77 (13%)	4	18
3	Н	610/701~(87%)	556~(91%)	54 (9%)	9	30
3	Ι	617/701~(88%)	530 (86%)	87 (14%)	3	16
All	All	4669/5452 (86%)	4182 (90%)	487 (10%)	10	24

All (487) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	6	GLU
1	А	11	THR
	a .:	7	



Mol	Chain	Res	Type
1	А	119	ARG
1	А	160	PHE
1	А	166	GLN
1	А	167	ASP
1	А	199	MET
1	А	203	GLU
1	А	204	TYR
1	А	206	THR
1	А	211	GLN
1	А	214	SER
1	А	217	LEU
1	А	219	GLN
1	А	220	ILE
1	А	221	ARG
1	А	222	ILE
1	А	225	LEU
1	А	226	SER
1	А	227	GLU
1	А	228	VAL
1	А	229	THR
1	А	230	GLN
1	А	231	ARG
1	А	253	MET
1	А	270	ILE
1	А	389	SER
1	А	397	ARG
1	А	401	ARG
1	А	412	VAL
1	А	415	LEU
1	А	443	PHE
1	В	61	MET
1	В	66	GLU
1	В	67	SER
1	В	68	LYS
1	В	119	ARG
1	B	160	PHE
1	В	199	MET
1	В	206	THR
1	В	209	ARG
1	В	211	GLN
1	В	213	LEU
1	В	217	LEU



Mol	Chain	Res	Type
1	В	218	SER
1	В	220	ILE
1	В	221	ARG
1	В	222	ILE
1	В	223	ASP
1	В	225	LEU
1	В	226	SER
1	В	227	GLU
1	В	253	MET
1	В	270	ILE
1	В	277	GLU
1	В	278	ASN
1	В	279	PRO
1	В	280	CYS
1	В	396	ARG
1	В	397	ARG
1	В	399	VAL
1	В	401	ARG
1	В	439	MET
1	В	450	VAL
1	В	530	ILE
1	G	8	GLN
1	G	11	THR
1	G	34	VAL
1	G	40	THR
1	G	41	GLU
1	G	71	HIS
1	G	74	LEU
1	G	75	ARG
1	G	84	ILE
1	G	119	ARG
1	G	160	PHE
1	G	167	ASP
1	G	171	GLN
1	G	172	LEU
1	G	173	SER
1	G	193	THR
1	G	194	VAL
1	G	195	ARG
1	G	200	LEU
1	G	203	GLU
1	G	206	THR



Mol	Chain	Res	Type
1	G	209	ARG
1	G	210	SER
1	G	211	GLN
1	G	213	LEU
1	G	218	SER
1	G	219	GLN
1	G	221	ARG
1	G	222	ILE
1	G	223	ASP
1	G	225	LEU
1	G	227	GLU
1	G	253	MET
1	G	255	LYS
1	G	270	ILE
1	G	277	GLU
1	G	280	CYS
1	G	282	LEU
1	G	396	ARG
1	G	397	ARG
1	G	399	VAL
1	G	401	ARG
1	G	443	PHE
1	J	8	GLN
1	J	11	THR
1	J	57	ARG
1	J	59	MET
1	J	75	ARG
1	J	82	LEU
1	J	119	ARG
1	J	146	GLU
1	J	160	PHE
1	J	167	ASP
1	J	169	PHE
1	J	171	GLN
1	J	172	LEU
1	J	173	SER
1	J	191	GLU
1	J	193	THR
1	J	194	VAL
1	J	195	ARG
1	J	196	GLU
1	J	201	TRP



Mol	Chain	Res	Type
1	J	204	TYR
1	J	205	ASN
1	J	206	THR
1	J	210	SER
1	J	211	GLN
1	J	213	LEU
1	J	214	SER
1	J	217	LEU
1	J	218	SER
1	J	219	GLN
1	J	222	ILE
1	J	223	ASP
1	J	225	LEU
1	J	227	GLU
1	J	253	MET
1	J	270	ILE
1	J	399	VAL
1	J	401	ARG
1	J	443	PHE
2	D	35	TRP
2	D	49	ILE
2	D	52	LEU
2	D	54	ILE
2	D	86	ARG
2	D	88	LEU
2	D	89	LYS
2	D	97	ASP
3	F	201	TYR
3	F	206	GLU
3	F	212	MET
3	F	218	GLN
3	F	220	GLU
3	F	223	LYS
3	F	328	LEU
3	F	336	LYS
3	F	339	VAL
3	F	345	LEU
3	F	346	LEU
3	F	349	LYS
3	F	351	ARG
3	F	355	PHE
3	F	357	LEU



Mol	Chain	Res	Type
3	F	358	GLU
3	F	364	ARG
3	F	369	THR
3	F	377	PHE
3	F	379	ASN
3	F	382	SER
3	F	384	SER
3	F	386	GLU
3	F	390	LEU
3	F	395	LYS
3	F	396	LEU
3	F	397	LYS
3	F	398	LYS
3	F	406	GLN
3	F	407	GLU
3	F	414	LYS
3	F	418	LEU
3	F	422	MET
3	F	423	GLN
3	F	425	LYS
3	F	459	LYS
3	F	462	CYS
3	F	468	SER
3	F	478	SER
3	F	480	SER
3	F	515	THR
3	F	521	LYS
3	F	522	CYS
3	F	523	ASN
3	F	524	ILE
3	F	546	ARG
3	F	547	GLN
3	F	548	LEU
3	F	593	GLN
3	F	613	PHE
3	F	619	GLU
3	F	620	THR
3	F	622	ILE
3	F	623	PRO
3	F	624	GLU
3	F	625	ARG
3	F	665	PHE



Mol	Chain	Res	Type
3	F	669	LEU
3	F	680	LYS
3	F	687	GLU
3	F	688	ARG
3	F	689	LYS
3	F	692	ARG
3	F	694	LYS
3	F	695	VAL
3	F	701	HIS
3	F	702	GLU
3	F	703	ILE
3	F	709	ARG
3	F	711	MET
3	F	712	LYS
3	F	716	LYS
3	F	748	LEU
3	F	750	GLU
3	F	751	ARG
3	F	752	GLU
3	F	753	TYR
3	Н	202	GLU
3	Н	209	PHE
3	Н	210	LEU
3	Н	211	GLU
3	Н	212	MET
3	Н	215	GLU
3	Н	218	GLN
3	Н	219	MET
3	Н	220	GLU
3	Н	223	LYS
3	Н	225	LEU
3	Н	377	PHE
3	Н	378	LEU
3	Н	380	LEU
3	Н	381	ASN
3	Н	383	ARG
3	Н	386	GLU
3	Н	389	SER
3	Η	390	LEU
3	Н	394	ASP
3	Н	395	LYS
3	Н	396	LEU



Mol	Chain	Res	Type
3	Н	420	ARG
3	Н	515	THR
3	Н	521	LYS
3	Н	522	CYS
3	Н	523	ASN
3	Н	524	ILE
3	Н	542	LYS
3	Н	547	GLN
3	Н	593	GLN
3	Н	613	PHE
3	Н	620	THR
3	Н	622	ILE
3	Н	625	ARG
3	Н	665	PHE
3	Н	669	LEU
3	Н	680	LYS
3	Н	687	GLU
3	Н	688	ARG
3	Н	689	LYS
3	Н	691	THR
3	Н	694	LYS
3	Н	695	VAL
3	Н	698	ASP
3	Н	701	HIS
3	Н	702	GLU
3	Н	703	ILE
3	Н	709	ARG
3	Н	716	LYS
3	Н	750	GLU
3	Н	754	LEU
3	Н	756	ARG
3	Η	757	THR
2	K	35	TRP
2	К	41	ASN
2	Κ	42	CYS
2	K	86	ARG
2	К	88	LEU
2	К	91	ARG
2	K	92	GLN
2	K	93	VAL
2	K	94	CYS
2	K	97	ASP



Mol	Chain	Res	Type
2	K	99	ARG
2	K	100	GLU
3	Ι	47	LYS
3	Ι	72	LYS
3	Ι	202	GLU
3	Ι	206	GLU
3	Ι	210	LEU
3	Ι	212	MET
3	Ι	213	SER
3	Ι	219	MET
3	Ι	220	GLU
3	Ι	223	LYS
3	Ι	225	LEU
3	Ι	248	VAL
3	Ι	249	MET
3	Ι	254	LYS
3	Ι	255	SER
3	Ι	257	GLU
3	Ι	339	VAL
3	Ι	346	LEU
3	Ι	349	LYS
3	Ι	351	ARG
3	Ι	353	ASP
3	Ι	356	LEU
3	Ι	357	LEU
3	Ι	377	PHE
3	Ι	379	ASN
3	Ι	381	ASN
3	Ι	383	ARG
3	Ι	384	SER
3	Ι	390	LEU
3	Ι	395	LYS
3	Ι	398	LYS
3	Ι	400	VAL
3	Ι	407	GLU
3	I	414	LYS
3	Ι	417	VAL
3	Ι	418	LEU
3	I	427	VAL
3	Ι	433	LYS
3	Ι	436	LEU
3	Ι	438	ARG



Mol	Chain	Res	Type
3	Ι	486	GLU
3	Ι	487	PHE
3	Ι	488	ARG
3	Ι	491	LEU
3	Ι	496	VAL
3	Ι	497	SER
3	Ι	498	LEU
3	Ι	515	THR
3	Ι	516	GLN
3	Ι	519	THR
3	Ι	521	LYS
3	Ι	546	ARG
3	Ι	547	GLN
3	Ι	593	GLN
3	Ι	613	PHE
3	Ι	619	GLU
3	Ι	622	ILE
3	Ι	624	GLU
3	Ι	625	ARG
3	Ι	665	PHE
3	Ι	669	LEU
3	Ι	680	LYS
3	Ι	687	GLU
3	Ι	688	ARG
3	Ι	689	LYS
3	Ι	691	THR
3	Ι	692	ARG
3	Ι	694	LYS
3	Ι	695	VAL
3	Ι	697	ASP
3	Ι	701	HIS
3	Ι	702	GLU
3	Ι	703	ILE
3	Ι	709	ARG
3	Ι	712	LYS
3	Ι	714	ARG
3	Ι	715	LYS
3	Ι	716	LYS
3	Ι	717	MET
3	Ι	731	LYS
3	Ι	735	LEU
3	Ι	748	LEU



Mol	Chain	Res	Type
3	Ι	750	GLU
3	Ι	751	ARG
3	Ι	753	TYR
3	Ι	754	LEU
3	Ι	756	ARG
2	L	35	TRP
2	L	41	ASN
2	L	42	CYS
2	L	67	GLU
2	L	86	ARG
2	L	88	LEU
2	L	91	ARG
2	L	96	LEU
2	L	98	ASN
2	L	99	ARG
2	L	100	GLU
3	С	43	GLU
3	С	47	LYS
3	С	203	GLU
3	С	328	LEU
3	С	330	SER
3	С	336	LYS
3	С	340	ASP
3	С	341	TYR
3	С	376	TYR
3	С	377	PHE
3	С	378	LEU
3	С	379	ASN
3	С	382	SER
3	С	383	ARG
3	С	390	LEU
3	С	395	LYS
3	С	398	LYS
3	С	400	VAL
3	C	403	LEU
3	C	404	THR
3	С	406	GLN
3	C	411	ILE
3	С	416	MET
3	C	417	VAL
3	С	419	PHE
3	С	422	MET



Mol	Chain	Res	Type
3	С	423	GLN
3	С	425	LYS
3	С	454	MET
3	С	455	ILE
3	С	456	SER
3	С	462	CYS
3	С	466	PHE
3	С	469	LYS
3	С	498	LEU
3	С	512	TYR
3	С	515	THR
3	С	516	GLN
3	С	521	LYS
3	С	522	CYS
3	С	523	ASN
3	С	524	ILE
3	С	542	LYS
3	С	544	SER
3	С	547	GLN
3	С	593	GLN
3	С	613	PHE
3	С	619	GLU
3	С	620	THR
3	С	621	ASP
3	С	622	ILE
3	С	625	ARG
3	С	627	LEU
3	С	665	PHE
3	C	669	LEU
3	С	680	LYS
3	С	687	GLU
3	C	688	ARG
3	C	689	LYS
3	C	691	THR
3	С	692	ARG
3	C	694	LYS
3	С	697	ASP
3	С	703	ILE
3	С	704	GLU
3	С	709	ARG
3	C	711	MET
3	С	716	LYS



Mol	Chain	Res	Type
3	С	728	GLN
3	С	729	GLN
3	С	731	LYS
3	С	735	LEU
3	С	748	LEU
3	С	750	GLU
3	С	751	ARG
3	С	752	GLU
3	С	753	TYR
3	С	754	LEU
3	С	757	THR
2	Е	35	TRP
2	Е	41	ASN
2	Е	42	CYS
2	Е	86	ARG
2	Е	88	LEU
2	Е	91	ARG
2	Е	92	GLN
2	Е	93	VAL
2	Е	94	CYS
2	Е	98	ASN
2	Е	99	ARG
2	Е	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	8	GLN
1	А	230	GLN
1	А	356	GLN
1	А	357	GLN
1	В	8	GLN
1	В	69	GLN
1	В	93	ASN
1	В	166	GLN
1	В	356	GLN
1	В	357	GLN
1	G	8	GLN
1	G	230	GLN
1	G	356	GLN
1	G	357	GLN
1	J	8	GLN



Mol	Chain	Res	Type
1	J	205	ASN
1	J	356	GLN
1	J	357	GLN
2	D	28	ASN
3	F	163	GLN
3	F	435	HIS
3	F	465	GLN
3	F	606	ASN
3	F	618	GLN
3	F	657	HIS
3	F	718	GLN
3	Н	163	GLN
3	Н	381	ASN
3	Н	465	GLN
3	H	481	ASN
3	Н	523	ASN
3	Н	606	ASN
3	Н	618	GLN
3	Н	657	HIS
3	Н	718	GLN
3	Н	729	GLN
2	K	41	ASN
2	K	47	ASN
3	Ι	163	GLN
3	Ι	465	GLN
3	Ι	481	ASN
3	Ι	606	ASN
3	Ι	618	GLN
3	Ι	657	HIS
2	L	28	ASN
2	L	41	ASN
2	L	47	ASN
2	L	98	ASN
3	С	163	GLN
3	С	379	ASN
3	С	434	GLN
3	С	443	ASN
3	С	481	ASN
3	С	523	ASN
3	С	547	GLN
3	С	606	ASN
3	С	618	GLN



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Mol	Chain	Res	Type
3	С	657	HIS
3	С	718	GLN
3	С	728	GLN
2	Е	28	ASN
2	Е	41	ASN
2	Е	47	ASN
2	Е	98	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34449. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 96



Y Index: 96



Z Index: 96

6.2.2 Raw map



X Index: 96

Y Index: 96

Z Index: 96

The images above show central slices of the map in three orthogonal directions.


6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 86



Y Index: 100



Z Index: 86

6.3.2 Raw map



X Index: 84

Y Index: 100

Z Index: 89

The images above show the largest variance slices of the map in three orthogonal directions.



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 117945 nm^3 ; this corresponds to an approximate mass of 106543 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.127 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.127 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	7.86	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	9.54	13.11	9.69	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.54 differs from the reported value 7.86 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34449 and PDB model 8H33. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0001).



9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9970	0.0700	_ 10
А	0.9980	0.0850	1.0
В	0.9980	0.0790	
С	0.9930	0.0520	
D	0.9990	0.0320	
E	0.9750	-0.0190	
F	0.9980	0.0840	
G	0.9990	0.0850	
Н	0.9990	0.0780	
I	0.9990	0.0810	0.0
J	0.9970	0.0570	<0.0
K	0.9670	0.0000	
L	0.9990	0.0280	

